

# Quantum Yields for the Photosensitized Formation of the Lowest Electronically Excited Singlet State of Molecular Oxygen in Solution

Francis Wilkinson

Department of Chemistry, University of Technology, Loughborough, Leicestershire, LE11 3TU, UK

and

W. Phillip Helman and Alberta B. Ross

Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556

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Quenching of excited singlet and triplet states of many substances by ground state molecular oxygen produces singlet oxygen, the lowest electronically excited singlet state of molecular oxygen,  $O_2(^1\Delta_g)$ . The fractions of singlet and triplet states quenched which produce singlet oxygen and the quantum yields of formation of singlet oxygen in fluid solutions have been critically compiled. Methods for determining yield parameters have been reviewed. Data have been compiled from the literature through 1991. Photosensitizers such as aromatic hydrocarbons, aromatic ketones and thiones, quinones, coumarins, fluoresceins, transition metal complexes, and heterocyclics are included in Table 1. Porphyrins and phthalocyanines are included in Table 2. Other materials which have been investigated for singlet oxygen production, such as dyes and drugs, are collected in Table 3 along with heterogeneous systems such as polymer-bound photosensitizers.

Key words: data compilation; energy transfer; excited states; oxygen; photosensitization; quantum yields; quenching; singlet oxygen; singlet states; solution; triplet states.

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## 1. Introduction

Ground state molecular oxygen,  $O_2$ , is well known to be highly reactive and essential for animal respiration. Its properties have been actively studied for more than 200 years. However the properties of its lowest electronically excited state have only been actively investigated during the last three decades. This is illustrated in the book entitled *Singlet Molecular Oxygen*<sup>1</sup> where Paul Schaap collects 28 Benchmark papers covering the period 1924–1973 which tell the story of the ‘discovery’ of singlet oxygen and many of the key steps taken towards present day understanding. There is strong evidence for the involvement of singlet oxygen, a powerful oxidant, in photo-sensitized oxidations, in photodynamic inactivation of viruses and cells, in phototherapy for cancer, in photocarcinogenesis, in the photodegradation of dyes and polymers and in the dye sensitization of the photodegradation of polymers. Much current interest in the chemical reactions of singlet oxygen stems from its potential as a photochemo-therapeutic agent.

The ground electronic state of molecular oxygen, which has zero angular momentum about the internuclear axis and contains two unpaired p electrons, has the group theoretical symbol  $^3\Sigma_g^-$ . The two electronically excited singlet states which arise from this same electron configuration but with spin pairing of the two electrons are the  $^1\Delta_g$  and the  $^1\Sigma_g^+$  states which lie 94 and 157 kJ mol<sup>-1</sup> respectively above the  $^3\Sigma_g^-$  ground state (see potential energy curves shown in Fig. 1). The electronic transitions  $^1\Delta_g \leftarrow ^3\Sigma_g^-$  and  $^1\Sigma_g^+ \leftarrow ^3\Sigma_g^-$  although highly forbidden are readily observed in absorption and emission in the upper atmosphere with zero-zero transitions at 1,269 and 762 nm and estimated radiative lifetimes of 64 min and 10 s, respectively.<sup>2,3</sup> The measured lifetimes in the gas phase and in solution are very much shorter than this. In fact, in condensed media, the lifetime of  $O_2^*(^1\Sigma_g^+)$  is so short that virtually nothing is known about its properties, and thus the term singlet oxygen is used throughout this review to refer to the  $^1\Delta_g$  state.

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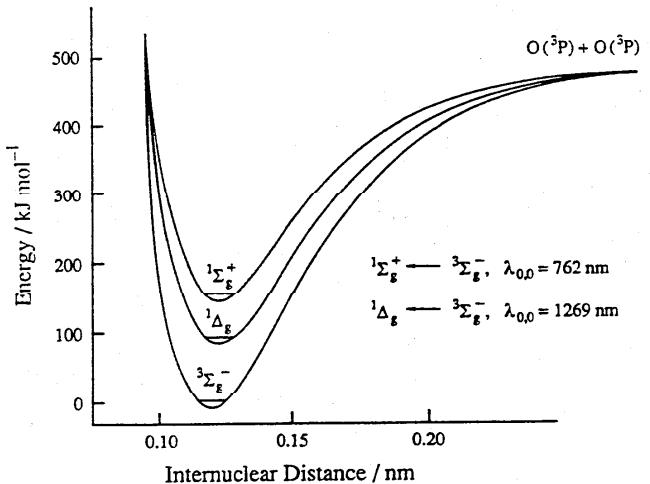


FIG. 1. Potential energy curves for molecular oxygen.

In 1963 Khan and Kasha<sup>4</sup> interpreted the red chemiluminescence of the hypochlorite-oxygen reactions as due to liberated singlet oxygen. Following the work of Ogryzlo *et al.*<sup>5,6</sup>, Khan and Kasha<sup>7</sup> gave a full spectroscopic correlation of the absorption and emission spectra in terms of the simultaneous transitions between the states shown in Fig. 2. Obviously the long-lifetime of  $^1\Delta_g$  even at one atmospheric pressure is such that two excited states collide

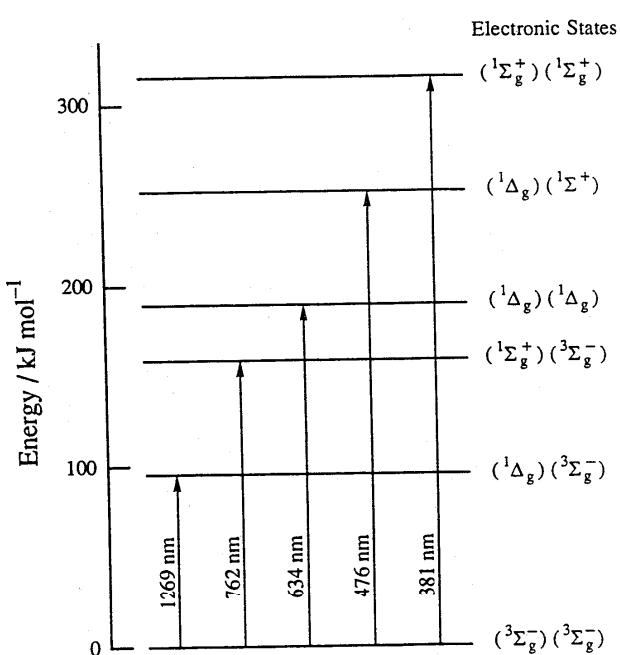


FIG. 2. Singlet state transitions and simultaneous pair-state transitions in molecular oxygen.

often enough for the simultaneous transition  ${}^1\Delta_g, {}^1\Delta_g \rightarrow {}^3\Sigma_g, {}^3\Sigma_g + h\nu$  to be seen.

Although singlet oxygen had been proposed as a possible intermediate in dye-sensitized photo-oxygenations by Kautsky as early as 1931<sup>8,9</sup> this was only firmly established following publications by Foote and Wexler<sup>10</sup> and Corey and Taylor<sup>11</sup> in 1964. A few years later a method for measuring the lifetime of singlet oxygen in solution was developed by Adams and Wilkinson<sup>12</sup> which made direct time measurements of the reaction of singlet oxygen with a reactive substrate, diphenylisobenzofuran following nanosecond laser photolysis enabling rate constants to be obtained for reactions of singlet oxygen. In 1976 Krasnovsky<sup>13</sup> used a mechanical phosphoroscope to detect the weak luminescence from  $O_2^*({}^1\Delta_g)$  at 1270 nm, thereby obtaining kinetic information concerning the reactions of singlet oxygen on millisecond timescales. However the development in the eighties of sensitive germanium photodiodes means that direct kinetic and relative yield studies of the phosphorescence of singlet oxygen are now routinely possible on timescales down to 1  $\mu$ s.

Numerous reviews<sup>14-22</sup> and several books<sup>23-25</sup> have recently been published on singlet oxygen and the field continues to grow dramatically. In 1981 we published a critical comprehensive compilation<sup>26</sup> on 'Rate Constants for the Decay and Reactions of the Lowest Electronically Excited State of Molecular Oxygen in Solution' which reported first order solvent deactivation rate constants for 50 different solvents and second order rate constants for the deactivation and chemical reaction of singlet oxygen

for 690 different compounds, from available data up to the end of 1978, including a few papers for 1979. We are in the process of updating this published compilation which we shall refer to as Paper I.<sup>26</sup> A considerable number of studies on singlet oxygen properties have been published in the last decade yielding hundreds of rate constants for reaction, quenching and decay but also increasingly hundreds of reports of the quantum yields of singlet oxygen production,  $\phi_\Delta$ , for many sensitizer-solvent systems. Since we did not collect data on quantum yields in Paper I<sup>26</sup> we have concentrated in this compilation on  $\phi_\Delta$  values. We have endeavored to keep the treatment consistent with Paper I<sup>26</sup> by using identical equation numbers and symbols wherever possible. In order to avoid too much duplication much reference is made to Paper I<sup>26</sup> especially when discussing singlet oxygen kinetics and reactions.

It is important to stress that photo-oxidation can arise as a result of several different mechanisms. Two major classes of photosensitized oxygenations have been designated as Type I and Type II<sup>27,28</sup>. In the former, the sensitizer interacts directly with the substrate resulting, for example, in either H-atom or electron transfer. The radicals so produced from the sensitizer react in the presence of oxygen to regenerate the sensitizers, while radicals produced from the substrate, for example, initiate free radical chain reactions, as observed in auto-oxidations, etc. Type II reactions involve the direct interaction of the excited sensitizer with oxygen which can give upon energy transfer singlet oxygen, which reacts with various substrates yielding Type II photosensitized reactions.<sup>28,29</sup>

## 2. Photosensitized Production of Singlet Oxygen in Solution

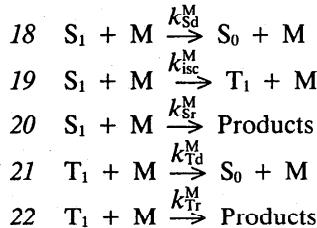
The method most frequently used for producing singlet oxygen in the laboratory is photosensitization (see Scheme 1). Both continuous irradiation and pulsed excitation studies have made much use of this method of production which also frequently occurs in nature. In this mechanism (Scheme 1) the lowest excited singlet and triplet states of the sensitizers are represented as  $S_1$  and  $T_1$  respectively and the ground electronic state by  $S_0$ . Any substrate which deactivates singlet oxygen by physical or chemical quenching is represented by  $M$  in Scheme 1. However, when quenching is known to be mainly by chemical reaction we shall use  $A$  to represent a reactive substrate and when a second 'reference' reactive substrate is employed we shall use  $A'$ . When the molecule is known to be a physical quencher with negligible reaction  $Q$  will be used in place of  $M$ . The singlet oxygen sensitizer even if it quenches singlet oxygen will be represented by  $S$  in place of  $M$ . When measurements are made relative to a reference sensitizer we shall label this  $S'$ . Thus  $M$  is a general symbol in Scheme 1 which may be replaced by  $A$ ,  $A'$ ,  $Q$ ,  $S$  or  $S'$  or any combination of these.

Scheme 1 is easily modified for self-sensitization also called photo-autoxidation where a substrate sensitizes its

Scheme 1

|    |   | Rate Constants         | Quantum Yields and Fractional Probabilities   |
|----|---|------------------------|---|
| 1  | $S_0 + h\nu \rightarrow S_1$                  | rate = $I_a$           |   |
| 2  | $S_1 \rightarrow S_0 + h\nu_F$                | $k_F$                  | $\phi_F = \frac{k_F}{k_{SD}}$   |
| 3  | $S_1 \rightarrow S_0$                         | $k_{ic}$               |   |
| 4  | $S_1 \rightarrow T_1$                         | $k_{isc}$              | $\phi_T = \frac{k_{isc}}{k_{SD}}$   |
| 5  | $S_1 + O_2^{\cdot} \rightarrow T_1 + ^1O_2^*$ | $k_{SD}^{O_2^{\cdot}}$ | $f_S^O = k_{SD}^{O_2^{\cdot}} / k_{SD}^{O_2}$   |
| 6  | $S_1 + O_2 \rightarrow T_1 + ^3O_2$           | $k_{SD}^{O_2}$         | $f_T^O = (k_{SD}^{O_2^{\cdot}} + k_{SD}^{O_2}) / k_{SD}^{O_2}$                          |
| 7  | $S_1 + O_2 \rightarrow S_0 + ^3O_2$           | $k_{SD}^{O_2}$         | $P_S^{O_2} = k_{SD}^{O_2}[O_2] / (k_{SD}^{O_2} + k_{SD}^{O_2}[O_2])$                    |
| 8  | $S_1 + O_2 \rightarrow \text{products}$       | $k_{Sr}^{O_2}$         | $1 - P_S^{O_2} = 1 / (1 + k_{SD}^{O_2}[O_2])$   |
|    |   |                        | $\phi_T^{O_2} = \phi_T(1 - P_S^{O_2}) + f_T^O P_S^{O_2}$                                |
| 9  | $T_1 \rightarrow S_0 + h\nu_P$                | $k_{TP}$               |   |
| 10 | $T_1 \rightarrow S_0$                         | $k_{Td}$               | $k_{TD} = (\tau_T^0)^{-1}$  |
| 11 | $T_1 + O_2 \rightarrow S_0 + ^1O_2^*$         | $k_{TD}^{O_2^{\cdot}}$ | $f_T^O = k_{TD}^{O_2^{\cdot}} / k_{TD}^{O_2}$   |
| 12 | $T_1 + O_2 \rightarrow S_0 + ^3O_2$           | $k_{TD}^{O_2}$         | $P_T^{O_2} = k_{TD}^{O_2}[O_2] / (k_{TD}^{O_2} + k_{TD}^{O_2}[O_2])$                    |
| 13 | $T_1 + O_2 \rightarrow \text{products}$       | $k_{Tr}^{O_2}$         |   |
| 14 | $^1O_2^* \rightarrow ^3O_2 + h\nu_P$          | $k_{\Delta P}$         | $f_P^O = k_{\Delta P} / (k_{\Delta P} + k_{\Delta d})$                                  |
| 15 | $^1O_2^* \rightarrow ^3O_2$                   | $k_{\Delta d}$         |   |
| 16 | $^1O_2^* + M \rightarrow \text{products}$     | $k_r^M$                | $f_r^M = k_r^M / (k_r^M + k_q^M)$   |
| 17 | $^1O_2^* + M \rightarrow ^1M + ^3O_2$         | $k_q^M$                |   |
|    |   |                        | $f_S^O = \text{fraction of } S_1 \text{ quenched by } O_2 \text{ which gives } ^1O_2^*$ |
|    |   |                        | $f_T^O = \text{fraction of } S_1 \text{ quenched by } O_2 \text{ which gives } T_1$     |
|    |   |                        | $f_T^T = \text{fraction of } T_1 \text{ quenched by } O_2 \text{ which gives } ^1O_2^*$ |
|    |   |                        | $P_S^{O_2} = \text{proportion of } S_1 \text{ quenched by } O_2$                        |
|    |   |                        | $P_T^{O_2} = \text{proportion of } T_1 \text{ quenched by } O_2$                        |

own photo-oxidation. However Scheme 1 does not include any of the possible reactions between the substrate M with the sensitizer singlet or triplet states  $S_1$  or  $T_1$  e.g.



These steps are not included in Scheme 1 since in most studies these reactions have been shown to be absent. In fact a major criterion for choosing a sensitizer is the absence of such complications. Other possible complications are the quenching or reaction of  $S_1$ ,  $T_1$  and  $^1O_2^*$  by products and other bimolecular reactions for example between  $^1O_2^*$  and  $T_1$  etc. These possibilities should be borne in mind especially when experimental conditions are varied markedly by using different types of sensitizers or highly reactive substrates, high concentrations, high light intensities etc. Fig. 3 shows pictorially the reaction scheme including all the steps 1-22.

The quantum yield of singlet oxygen production, via sensitization  $\phi_\Delta$ , is given by the sum of contributions due to oxygen quenching of  $S_1$  and  $T_1$  i.e.

$$\phi_\Delta = \phi_\Delta(S_1) + \phi_\Delta(T_1).$$

$\phi_\Delta$  depends on the concentration of oxygen and in the presence of oxygen quenching of both  $S_1$  and  $T_1$ , it follows from the steps shown in Scheme 1 (see Appendix 12.1.1 for derivation) that

$$\phi_\Delta = P_S^{O_2} f_S^O + \phi_T^{O_2} P_T^{O_2} f_T^T = P_S^{O_2} f_S^O + P_S^{O_2} f_T^{O_2} P_T^{O_2} f_T^T + \phi_T(1 - P_S^{O_2}) P_T^{O_2} f_T^T \quad (1)$$

which can be written as

$$\phi_\Delta = \phi_T P_T^{O_2} f_T^T + P_S^{O_2} \{ f_S^O + P_T^{O_2} f_T^T (f_T^{O_2} - \phi_T) \}.$$

When  $E_{S_1} - E_{T_1} \ll E_\Delta$ ,  $k_{SD}^{O_2} \rightarrow 0$  and thus sensitization is just by the triplet state, Eq. (1) becomes

$$\phi_\Delta = \phi_T P_T^{O_2} f_T^T = \phi_T(1 - P_S^{O_2}) P_T^{O_2} f_T^T + P_S^{O_2} f_T^{O_2} P_T^{O_2} f_T^T.$$

When the lifetime of  $S_1$  is such that  $k_{SD} \gg k_{SD}^{O_2}[O_2]$  a further simplification occurs and

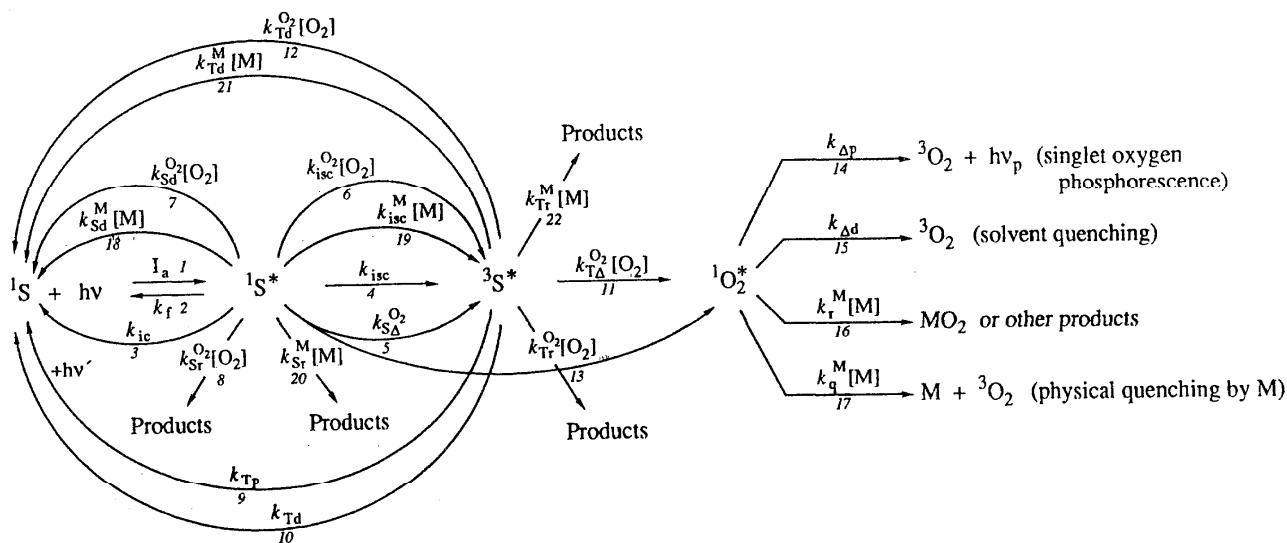


FIG. 3. Pictorial representation of full kinetic scheme [steps 1 to 22, see text] for photosensitized oxidation involving singlet oxygen. S = Sensitizer, M = Substrate.

$$\phi_\Delta = \phi_T P_T^{O_2} f_\Delta^T.$$

For many molecules, triplet lifetimes are long and oxygen quenching is very efficient. Thus even air saturated solutions have  $P_T^{O_2} = 1$ . In this case, in the absence of singlet state quenching by oxygen,

$$\phi_\Delta = \phi_T f_\Delta^T.$$

Various methods are available for measuring the quantum yield of singlet oxygen production and these will be discussed in Section 4.

### 2.1. Sensitized Production by Pulsed Radiolysis

When a high energy electron beam is passed through liquid benzene and some other solvents a high yield of excited states can be formed. Since the lifetimes of singlet and triplet states of benzene are only a few nanoseconds in neat benzene, quenching by dissolved oxygen does not produce much singlet oxygen. However, in the presence of a high concentration of a triplet energy acceptor, energy transfer to and then from its triplet state to oxygen yields singlet oxygen. For example, on pulsed radiolysis of benzene containing  $10^{-2}$  mol L<sup>-1</sup> naphthalene, triplet benzene is intercepted by naphthalene to give triplet naphthalene which is quenched by oxygen and enough singlet oxygen is produced to enable its properties to be probed using the technique of pulsed radiolysis.<sup>30</sup>

## 3. Methods for Studying Kinetics of the Reactions of Singlet Oxygen.

### 3.1. Phosphorescence Decay

Although the phosphorescence from singlet oxygen is highly forbidden and it occurs in the infrared region of the spectrum which presents many difficulties for experimentalists, it is now possible to detect the decay of singlet oxygen luminescence from very dilute solutions of sensitizers.<sup>31-37</sup> These kinds of measurements have enabled much more direct determinations of the lifetime of singlet oxygen than the indirect methods reported earlier.<sup>26</sup> If the logarithm of the phosphorescence intensity is plotted as a function of time then the slope equals the decay constant, given by:

$$k_D = k_\Delta + \Sigma k_M [M], \quad (2)$$

where M represents any molecule including the sensitizer which quenches singlet oxygen (via a physical process or a chemical reaction). Several workers<sup>38,39</sup> have measured  $k_D$  as a function of sensitizer concentration which enables both  $k_\Delta$  and the bimolecular rate constant for singlet oxygen quenching by the sensitizer  $k_s$  to be obtained. When a decay constant for singlet oxygen is measured in the presence of a sensitizer we shall use  $k_d = k_\Delta + k_s [S]$  for the decay constants. It is often assumed or demonstrated that under many experimental conditions  $k_d = k_\Delta$ ; how-

ever this is not always the case. Occasionally the value of  $k_d$  is obtained by measuring  $k_d$  as a function of [S] and extrapolating to  $[S] = 0$ .<sup>38</sup> This procedure is to be recommended.

### 3.2. Time Dependent Thermal Lensing due to Singlet Oxygen Decay

The absorption of even part of the energy in a laser pulse gives rise to local temperature changes in gases or liquids. This leads to changes in density and refractive index which causes the system to act as a diverging lens.<sup>40</sup> Time resolved thermal lensing (TL) due to release of energy by decaying excited states can be used to measure lifetimes of singlet oxygen in the range 0.1 to 100  $\mu\text{s}$ . A continuous laser beam used as a probe source is dispersed by the thermal lens reducing the light reaching a photodiode through a pinhole. The photodiode signal gives the relative magnitudes of heat contributions ( $U$ ) for fast and slow non-radiative processes relative to the acoustic transit time. The time dependence of the slow process gives rate information. The TL signal at time  $t$  is defined as

$$U(t) = \frac{V_0 - V(t)}{V_0} \quad (3)$$

where  $V(t)$  is the time dependent voltage generated by the detector and  $V_0$  is the value before excitation by the pump laser. Following the sensitized production of  ${}^1\text{O}_2^*$ ,  $\Delta U = U_{\text{total}} - U_{\text{fast}}$  decays exponentially with the decay constant  $k_D$  given by Eq. (2) (See also Section 4.2.2).

### 3.3 Time Dependent Acceptor Disappearance

#### 3.3.1. Following Pulsed Excitation of a Sensitizer

This method is discussed in detail in Paper I.<sup>26</sup> To summarize according to the mechanism given in Scheme 1, in this case with  $M = A$ , since we are discussing a reactive substrate, it follows that

$$-\frac{d[A]}{dt} = k_r^A [A][{}^1\text{O}_2^*].$$

Following pulsed excitation in aerated solutions most singlet and triplet states have decayed within 1  $\mu\text{s}$  and then

$$-\frac{d[{}^1\text{O}_2^*]}{dt} = (k_d + k_A[A])[{}^1\text{O}_2^*]$$

and thus

$$-d[A] = k_r^A [A][{}^1\text{O}_2^*]_{t=0} [\exp - (k_d t + \int_0^t k_A[A] dt)]. \quad (4)$$

Equation (4) has been treated slightly differently by Adams and Wilkinson<sup>12</sup>, by Young *et al.*<sup>41</sup> and by Merkel and Kearns<sup>42</sup> as explained in Paper I.<sup>26</sup> However for very small changes in [A] (i.e. less than 10%) all of these treatments effectively put  $[A] = [A]_{\text{av}}$ , the average value of [A], and integrate Eq. (4) taking  $k_D = k_d + k_A[A]_{\text{av}}$  to give

$$[A]_t - [A]_\infty = \frac{k_r^A [{}^1\text{O}_2^*]_{t=0} [A]_{\text{av}}}{k_D} e^{-k_D t}. \quad (5)$$

Since the change in concentration of A is proportional to  $\Delta A$ , the change in absorbance by the oxidizable acceptor at some convenient wavelength; i.e.  $[A]_t - [A]_\infty = \Delta A / \epsilon l$ , where  $\epsilon$  is the extinction coefficient and  $l$  the analyzing path-length. It follows from Eq. (5) that

$$\ln \Delta A = -k_D t + \text{const} \quad (6)$$

and a plot of  $-\ln \Delta A$  vs.  $t$  should have a slope equal to  $k_D = k_d + k_A[A]_{\text{av}}$ . Thus by varying  $[A]_{\text{av}}$  values of  $k_d$  and  $k_A$  can be determined. If  $k_A$  is only partly due to chemical quenching and partly due to physical quenching, the value of  $k_A$  obtained will be the rate constant due to the combination of both processes; i.e.  $k_A = k_r^A + k_q^A$ . Thus when A acts both as a physical and as a chemical quencher, the value of  $k_A$  obtained is the total rate constant for quenching due to both processes. The acceptor used in most studies of this type is the original one chosen by Adams and Wilkinson,<sup>12</sup> namely 1,3-diphenylisobenzofuran, DPBF. In the presence of several possible singlet oxygen quenchers (i.e. Scheme 1 with  $M = A, S$  and  $Q$ ), we have

$$k_D = k_d + k_s[S] + k_Q[Q] + k_A[A]. \quad (9)$$

Measurement of  $k_D$  as a function of [Q] keeping [S] and [A] constant allows values of  $k_Q$  to be obtained. N.B. If  $k_Q$  is only partly due to physical quenching and a small part is due to reaction, the value of  $k_Q$  obtained will be the total rate constant for quenching due to both processes.

A variation on this method has been reported by Matheson, *et al.*<sup>43,44</sup> in which singlet oxygen is directly generated by absorption of the output at 1065 nm of a pulsed Nd-glass laser by oxygen dissolved under pressure (up to 130 atm) in 1,1,2-trichlorotrifluoroethane (Freon 113) and the disappearance of the singlet oxygen acceptor DPBF was monitored. Farmilo and Wilkinson<sup>45</sup> have developed a method for measuring singlet oxygen decay which monitors absorption by triplet  $\beta$ -carotene,  ${}^3\text{C}^*$ , formed by energy transfer from singlet oxygen in aerated solutions containing a sensitizer and a low concentration of  $\beta$ -carotene. Under appropriate conditions the decay of absorption at 520 nm due to  ${}^3\text{C}^*$  mirrors the singlet oxygen decay yielding values of  $k_D$ . Paper I<sup>26</sup> describes these methods in detail (see Eqs. (7)–(12) given there).

#### 3.3.2. Monitoring Sensitized Photo-oxidations by Consumption of Reactants or Appearance of Products Under Steady-State Conditions

Many photosensitized reactions of a single substrate A have been carried out under conditions such that no quenching by A of the sensitizer singlet or triplet states occurs, in which case the mechanism is as given in Scheme 1, with  $M = A$ . For continuous irradiation,

$$-\frac{d[A]}{dt} = -\frac{d[O_2]}{dt} = \frac{d[P]}{dt} = k_r^A [{}^1O_2^*]_{ss}[A] \quad (13)$$

and the steady-state approximation can be applied to  $S_1$ ,  $T_1$  and  ${}^1O_2^*$  (See Appendix 1, Sec. 12.1.1) to give

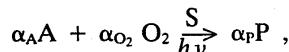
$$\phi_{ox} = \frac{r_{ox}}{I_a} = \frac{\phi_\Delta k_r^A [A]}{k_d + k_A [A]} = \phi_\Delta p_A, \quad (14)$$

where  $p_A$  is the fraction of the  $O_2^*({}^1\Delta_g)$  formed which reacts with A. The rate of oxygenation may be followed by determining the rate of production of some product and/or the rate of disappearance of either the substrate A and/or of oxygen. All three have been used. N.B. It follows from Eq. (14) that when  $k_d \gg k_A[A]$  or  $k_A[A] \gg k_d$  the rate of oxygenation will be first or zero order respectively with respect to A. Equation (14) can be rearranged to give

$$r_{ox}^{-1} = (I_a \phi_\Delta f_r^A)^{-1} \left[ 1 + \frac{k_d}{k_A [A]} \right] \quad (15)$$

where  $f_r^A = k_r^A/k_A$  is the fraction of reactive quenching of singlet oxygen by A.

Most reactive substrates (A) react with singlet oxygen with unit stoichiometry as implied in Eqs. (13) to (15) which apply when each time a molecule of  ${}^1O_2^*$  reacts it leads to the consumption of one molecule of A and one of  $O_2$  and produces one molecule of the product P. If there are stoichiometry factors  $\alpha$  different from unity, i.e. the overall reaction is given by the equation



then

$$r_{ox} = -\frac{1}{\alpha_A} \frac{d[A]}{dt} = -\frac{1}{\alpha_{O_2}} \frac{d[O_2]}{dt} = \frac{1}{\alpha_P} \frac{d[P]}{dt}$$

and Eqs. (14) and (15) still apply. If however the rate of the reaction is monitored by observing the rate of consumption of a reactive substrate such as thiourea where  $\alpha = 2$  and this rate is not divided by  $\alpha = 2$ , then  $\alpha f_r^A$  instead of  $f_r^A$  appears in Eqs. (14) and (15). This adjustment needs to be made whenever unit stoichiometry does not apply.

According to Eq. (15) linear plots of  $r_{ox}^{-1}$  or  $\phi_{ox}^{-1}$  vs.  $[A]^{-1}$  should give

$$\frac{\text{slope}}{\text{intercept}} = \frac{k_d}{k_A} = \beta_A,$$

where  $\beta_A = k_d/k_A$  represents the concentration at which the decay of singlet oxygen in the solvent sensitizer system equals the decay due to quenching by A by both physical and chemical paths (steps 16 and 17); i.e. it is the half-quenching concentration. N.B. Eq. (15) only predicts a linear relationship if there is (i) constant light intensity, (ii) constant absorption by the sensitizer and with no absorption by A although this could be allowed for, and (iii) a constant oxygen concentration in the solution. For ex-

amples see Refs. 46–48 and Paper I<sup>26</sup> where hundreds of  $\beta$  values are given.

Several modifications on this theme are possible including the addition of quenchers which allow values of  $\beta_Q = k_d/k_Q$  to be obtained. (For details see Paper I<sup>26</sup> and Eqs. (16)–(26) given there). If values of  $k_d$  are available  $\beta$  values can be converted into rate constants  $k_A$  and  $k_Q$ . Usually the rate constant obtained in this way is the sum of  $k_r$  and  $k_q$  contributions; however these can be separated as discussed below.

### 3.3.3. Separation of $k_r$ and $k_q$

Methods which have been used to separate  $k_r$  and  $k_q$  values usually involve the direct measurement of the quantum yields of oxygenation,  $\phi_{ox}$ . For example at high concentrations of A such that  $k_A [A] \gg k_d$ , it follows from Eq. (14) that

$$(\phi_{ox})_{[A] \rightarrow \infty} = \phi_\Delta f_r^A. \quad (27)$$

Alternatively at low values of [A] when  $k_d \gg k_A [A]$  Eq. (14) gives

$$\phi_{ox} = \frac{\phi_\Delta k_r^A [A]}{k_d}. \quad (28)$$

Thus measurement of relative values of  $\phi_{ox}$  or  $r_{ox}$ , under identical conditions at either of these limits allows the evaluation of relative values of  $k_r^A$ . It follows from Eqs. (27) and (28) that measurement of  $\phi_{ox}$  together with a knowledge of  $\phi_\Delta$  and  $k_d$  or  $\beta_A$  allows values of  $k_r^A$  or  $f_r^A$  to be determined. Often the limiting yield of oxygenation of a very reactive acceptor (e.g.  $\alpha$ -terpinene or 2,5-dimethylfuran (2,5-DMF = A')) for which  $f_r^{A'}$  is close to unity (i.e.  $k_r^{A'} \gg k_q^{A'}$ ) is used as a reference substrate to give values of  $\phi_\Delta$  and hence  $k_r^A$  for other additives.<sup>49,50</sup> Gollnick and Griesbeck<sup>51</sup> have for example measured the rates of oxygen consumption of various substrates relative to that of 2,5-DMF at concentrations greater than  $4 \times 10^{-5}$  mol L<sup>-1</sup> in methanol. Since  $k_r^{A'} \gg k_q^{A'}$ ,  $f_r^{A'} = 1$  and the concentration is such that  $k_A [A'] \gg k_d$  and thus  $r_{ox}^{A'} = I_a \phi_\Delta$ , and

$$\frac{r_{ox}^{A'}}{r_{ox}^A} = \frac{(k_r^A + k_q^A)[A] + k_s[S] + k_\Delta}{k_r^A [A]}$$

or

$$\frac{r_{ox}^{A'}}{r_{ox}^A} = \left[ 1 + \frac{k_q^A}{k_r^A} \right] + \left[ \frac{k_\Delta}{k_r^A} + \frac{k_s[S]}{k_r^A} \right] \frac{1}{[A]}. \quad (29)$$

Plots of  $r_{ox}^{A'}/r_{ox}^A$  versus  $[A]^{-1}$  are linear and values of  $k_q^A/k_r^A$  can be determined from the intercepts. Variations in the slope of such plots as a function of the sensitizer concentration allow values of  $k_s/k_r^A$  and  $k_\Delta/k_r^A$  to be determined. If  $k_\Delta$  is known then  $k_r^A$ ,  $k_s$  and  $k_q^A$  can be determined; e.g. see Ref. 50 and also Paper I<sup>26</sup> and Eqs. (30)–(37) given there for various other methods.

#### 4. Methods for Determining the Sensitized Yields of Singlet Oxygen Production

According to Scheme 1, as outlined in Sec. 2 and as derived in Appendix 1, Sec. 12.1.1, the quantum yield of singlet oxygen production from quenching of both singlet and triplet states of the sensitizer is given by Eq. (1); i.e.

$$\phi_{\Delta} = \phi_T P_T^{Q_2} f_{\Delta}^T + P_S^{Q_2} \{f_{\Delta}^S + P_T^{Q_2} f_{\Delta}^T (f_T^{Q_2} - \phi_T)\}. \quad (1)$$

It follows from Scheme 1 that there would be two molecules of  ${}^1O_2^*$  produced for every photon absorbed if oxygen were to quench all the singlet states of a sensitizer to give  ${}^1O_2^*$  and if in addition all triplet states were quenched by oxygen with 100% efficiency to give  ${}^1O_2^*$ . This is apparent from Eq. (1) since  $\phi_{\Delta} = 2$  when  $P_S^{Q_2} = P_T^{Q_2} = f_{\Delta}^T = f_{\Delta}^S = f_T^{Q_2} = 1$ . This limit is approached for some systems (see some of the limiting values for Entry numbers 1.19 and 1.25 in Table 1) at high oxygen concentrations. At room temperatures air-saturated solutions of most organic solvents contain  $(1-3) \times 10^{-3}$  mol L<sup>-1</sup> of dissolved oxygen, while in water, ethylene glycol and glycerol, the values are much less: 2.9, 1.2 and  $0.7 \times 10^{-4}$  mol L<sup>-1</sup>, respectively. Typically the rate constants for quenching of excited singlet states by oxygen in nonviscous solvents are in the range  $(2-4) \times 10^{10}$  L mol<sup>-1</sup> s<sup>-1</sup>. Thus  $k_{S_1}^{Q_2} = 6 \times 10^7$  s<sup>-1</sup> and  $3 \times 10^8$  s<sup>-1</sup> in air- and oxygen-saturated solutions. It follows that singlet states with lifetimes of 16.7 ns and 3.3 ns for air and oxygen saturated solutions will have  $P_S^{Q_2} = 0.5$ ; i.e. half the excited singlet states would be quenched by oxygen. Compounds with singlet state lifetimes twenty times longer or shorter than these will have  $P_S^{Q_2} = 0.95$  and 0.05 respectively. In general therefore when excited singlet state lifetimes are less than 0.15 ns  $P_S^{Q_2} < 0.05$ . This is often the case for example for aromatic ketones with lowest singlet states which are n,π\* states. However the singlet states of aromatic hydrocarbons are often such that  $P_S^{Q_2}$  is critically dependent on oxygen solubility and thus on solvent, viscosity, temperature, etc, as are therefore  $\phi_{\Delta}$  values. As far as oxygen quenching of triplet states is concerned,  $k_{T_1}^{Q_2}$  values are usually one order of magnitude less than  $k_{S_1}^{Q_2}$ , so when the triplet state lifetimes are >3.3 μs or >16.6 μs then  $P_T^{Q_2} > 0.95$  for oxygen and air saturated solutions respectively. When  $P_T^{Q_2} = 1$ , Eq. (1) becomes

$$\phi_{\Delta} = \phi_T f_{\Delta}^T + P_S^{Q_2} \{f_{\Delta}^S + f_{\Delta}^T (f_T^{Q_2} - \phi_T)\} \quad (38)$$

or equally well in terms of [O<sub>2</sub>] and the Stern-Volmer constant for singlet quenching by O<sub>2</sub>,  $K_{SV}$

$$\phi_{\Delta} = \frac{\phi_T f_{\Delta}^T + K_{SV}[O_2] (f_{\Delta}^S + f_{\Delta}^T f_T^{Q_2})}{1 + K_{SV}[O_2]}. \quad (38)$$

Since

$$\frac{F^{\circ}}{F} = 1 + K_{SV}[O_2],$$

where  $F^{\circ}$  and  $F$  represent the sensitizer fluorescence intensity in the absence and presence of oxygen another form of Eq. (38) is

$$\frac{F^{\circ}}{F} \phi_{\Delta} = \phi_T f_{\Delta}^T + (f_{\Delta}^S + f_{\Delta}^T f_T^{Q_2}) \left[ \frac{F^{\circ}}{F} - 1 \right]. \quad (38)$$

This form of Eq. (38) is often combined with Eq. (14) to give

$$\frac{F^{\circ} \phi_{ox}}{F p_A} = \phi_T f_{\Delta}^T + (f_{\Delta}^S + f_{\Delta}^T f_T^{Q_2}) \left[ \frac{F^{\circ}}{F} - 1 \right]. \quad (14,38)$$

Thus a plot of

$$\left( \frac{F^{\circ} \phi_{ox}}{F p_A} \right) \text{ versus } \left[ \frac{F^{\circ}}{F} - 1 \right]$$

or equally well

$$\phi_{ox}(1 + K_{SV}[O_2]) / p_A \text{ versus } K_{SV}[O_2]$$

will give a straight line with an intercept equal to  $\phi_T f_{\Delta}^T$  and a slope of  $(f_{\Delta}^S + f_{\Delta}^T f_T^{Q_2})$ . In addition often  $f_T^{Q_2}$  is, perhaps too readily, assumed equal to one in order to allow the sum  $f_{\Delta}^S + f_{\Delta}^T$  to be obtained.

Often the contribution to the singlet oxygen yield from singlet state quenching is negligible; this is certainly so when  $E_{S_1} - E_{T_1} \ll E_{\Delta}$ . In this case  $f_{\Delta}^S = 0$  and Eq. (1) becomes:

$$\phi_{\Delta} = \phi_T P_T^{Q_2} f_{\Delta}^T = \phi_T P_T^{Q_2} f_{\Delta}^T + P_S^{Q_2} P_T^{Q_2} f_{\Delta}^T (f_T^{Q_2} - \phi_T). \quad (39)$$

If in addition to  $f_{\Delta}^S = 0$ ,  $P_T^{Q_2} = 1$  or if one divides  $\phi_{\Delta}$  by  $P_T^{Q_2}$  to correct for total triplet quenching, the triplet yield is still modified by O<sub>2</sub> and

$$\phi_{\Delta} = \phi_{\Delta} / P_T^{Q_2} = \phi_T f_{\Delta}^T = \phi_T f_{\Delta}^T + P_S^{Q_2} f_{\Delta}^T (f_T^{Q_2} - \phi_T). \quad (39)$$

Although  $f_T^{Q_2}$  has been shown in some cases to be close to unity, in other cases this is not so and the assumption that  $f_T^{Q_2} = 1$  should be checked. However when  $f_T^{Q_2} = 1$  Eq. (1) becomes:

$$\phi_{\Delta} = \phi_T P_T^{Q_2} f_{\Delta}^T + P_S^{Q_2} \{f_{\Delta}^S + P_T^{Q_2} f_{\Delta}^T (1 - \phi_T)\} \quad (40)$$

and when  $f_T^{Q_2} = P_T^{Q_2} = 1$

$$\phi_{\Delta} = \phi_T f_{\Delta}^T + P_S^{Q_2} \{f_{\Delta}^S + f_{\Delta}^T (1 - \phi_T)\}.$$

When there is negligible oxygen quenching of S<sub>1</sub> which occurs for short lived singlet states as explained above (i.e. when  $P_S^{Q_2} = 0$ ) Eq. (1) becomes

$$\phi_{\Delta} = \phi_T P_T^{Q_2} f_{\Delta}^T \quad (41)$$

and Eq. (41) simplifies further if in addition  $P_T^{Q_2} = 1$  and the value of  $\phi_{\Delta}$  corrected for total triplet quenching is given by

$$\phi_{\Delta}^T = \phi_{\Delta}/P_T^{Q_2} = \phi_{\Delta} f_{\Delta}^T. \quad (42)$$

All the forms of Eq. (1) given above, i.e. Eqs. (38)–(42) have been used in the literature. N.B. When excitation is by pulse radiolysis, yields are measured as  $G$  values, where  $G(^1\text{O}_2^*)$  for example is the number of singlet oxygen molecules produced per 100 eV of absorbed radiation. Gorman *et al.*<sup>30</sup> have shown that under the appropriate conditions (e.g. when  $P_S^{Q_2} = 0$ , and  $P_T^{Q_2} = 1$ ), Eq. (42) can be used with  $G(^1\text{O}_2^*)$  and  $G(^3\text{S}^*)$  scavenged by  $\text{O}_2$  replacing  $\phi_{\Delta}^T$  and  $P_T^{Q_2}\phi_{\Delta}$  respectively.

It is useful to place sensitizers into one of three categories (as suggested in Ref. 52). We prefer not to use categories I, II and III as suggested in Ref. 52 in order to avoid confusion with type I and type II photo-oxidations. We use Type T for molecules where, in the range of concentration of oxygen normally employed, there is no singlet state quenching by  $\text{O}_2$  (i.e.  $P_S^{Q_2} = 0$ ) and for which therefore Eqs. (41) and (42) hold. We use Type ST for sensitizers which have singlet and triplet states which may both be quenched by oxygen to give  ${}^1\text{O}_2^*$ , i.e. type ST sensitizers have  $P_S^{Q_2} \neq 0$  and  $E_{S_1} - E_{T_1} \geq E_{\Delta}$ . Equations (1), (38), (14,38) and (39) apply to type ST sensitizers and at the limit when  $P_T^{Q_2} = P_S^{Q_2} = 1$ , i.e.  $[\text{O}_2] \rightarrow \infty$ ,

$$\phi_{\Delta}^{\text{ST}} = f_{\Delta}^S + f_{\Delta}^T f_T^{Q_2}, \text{ for type ST sensitizers.}$$

We use Type TC for those sensitizers with singlet states which are quenched by  $\text{O}_2$  but which have  $E_{S_1} - E_{T_1} \ll E_{\Delta}$  and which therefore have  $f_{\Delta}^S = 0$  and have triplet yields ( $\phi_T^{Q_2}$ ) and quantum yields of singlet oxygen production ( $\phi_{\Delta}$ ) which depend on the amount of singlet quenching by oxygen. The triplet yield of the sensitizer changes according to the extent of singlet state quenching by oxygen and the extent of catalysed triplet states produced thereby. For type TC sensitizers Eq. (39) holds when  $P_T^{Q_2} = 1$  and when in addition  $P_S^{Q_2} = 1$  the limiting value for  $[\text{O}_2] \rightarrow \infty$  is

$$\phi_{\Delta}^{\text{TC}} = f_{\Delta}^T f_T^{Q_2}, \text{ for type TC sensitizers.}$$

For type TC sensitizers  $\phi_{\Delta}^{\text{ST}}$  can be greater or lower than  $\phi_{\Delta}^T$  depending on whether  $f_T^{Q_2}$  is greater or less than  $\phi_T^{Q_2}$ . For type T sensitizers where contributions due to oxygen quenching of  $S_1$  are negligible (e.g., many aromatic ketones), it follows from Eq. (41) that

$$\frac{1}{\phi_{\Delta}} = \frac{1}{\phi_T f_{\Delta}^T} \left[ 1 + \frac{k_{\text{TD}}}{k_{\text{TQ}}^{Q_2} [\text{O}_2]} \right]$$

and the intercept of linear plots of  $\phi_{\Delta}^{-1}$  vs.  $[\text{O}_2]^{-1}$  gives  $\phi_{\Delta}^T = \phi_T f_{\Delta}^T$  i.e. the value at the limit where  $P_T^{Q_2} \rightarrow 1$ . N.B. In such cases one would have to make studies at much higher oxygen pressures to reach the limit where  $P_S^{Q_2}$  also equals unity. Several workers evaluate  $P_T^{Q_2}$  and/or  $P_S^{Q_2}$  and are thus able to calculate values of  $\phi_{\Delta}^T$  and  $\phi_{\Delta}^{\text{ST}}$  defined above. In the tables such values are labelled with superscripts (e.g.  $0.5^T$  and  $0.7^{\text{ST}}$ ) although some of these limiting values have not been obtained in practice but only by extrapolation.

## 4.1. Photo-oxidation Studies

### 4.1.1. Steady-State Irradiation

Many authors have reported values for  $\phi_{\Delta}$  obtained by measuring quantum yields of photo-oxidation under steady-state conditions. Equation (14) derived from Scheme 1 with  $M = A$  can be written in several forms i.e.

$$\phi_{\text{ox}} = \frac{\phi_{\Delta} k_r^A [A]}{k_d + k_A [A]} = \frac{\phi_{\Delta} f_r^A [A]}{\beta_A + [A]} = \phi_{\Delta} p_A \quad (14)$$

where  $p_A$  is the proportion of  ${}^1\text{O}_2^*$  formed which reacts. This equation has also been used to determine  $\phi_{\Delta}$  using pulsed laser excitation<sup>53</sup> and in pulsed radiolysis experiments only with  $G$  values in place of quantum yields.<sup>30</sup>

At high concentrations of  $[A]$  such that  $k_d \ll k_A [A]$

$$(\phi_{\text{ox}})_{[A] \rightarrow \infty} = \phi_{\Delta} f_r^A. \quad (27)$$

Often it is assumed that  $f_r^A = 1$  for very reactive substrates. Certainly if several substrates give the same limiting yield,<sup>54</sup> it is reasonable to assume  $f_r^A = 1$ . Unless otherwise stated in the Table 'Comments'  $f_r^A$  has been assumed to be unity for all  $A$ . The stoichiometry of the overall reaction also needs to be established (see Section 3.3.2). Equations (14) and (27) are often used to determine  $\phi_{\Delta}(S)$  for one sensitizer relative to a 'known' value of  $\phi_{\Delta}(S')$  for a reference sensitizer,  $S'$ , since for measurements under identical conditions Eq. (14) gives

$$\frac{\phi_{\Delta}(S)}{\phi_{\Delta}(S')} = \frac{\phi_{\text{ox}}(S)}{\phi_{\text{ox}}(S')}. \quad (43)$$

Of course the ratio of any measurement directly proportional to  $\phi_{\text{ox}}$  can be used in Eq. (43).

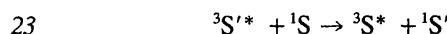
When low concentrations of acceptor are used such that  $k_d \gg k_A [A]$  Eq. (14) yields

$$-\frac{d[A]}{dt} = \frac{I_{\text{abs}} \phi_{\Delta} k_r^A [A]}{k_d}$$

cf. Eq. (28) and a first order dependence of the disappearance of  $A$  with time is observed. The slopes of first order plots measured under identical conditions allow relative values of  $\phi_{\Delta}$  to be obtained since

$$\frac{\phi_{\Delta}(S)}{\phi_{\Delta}(S')} = \frac{-d(\ln A)/dt}_S \frac{-d(\ln A)/dt}_{S'}. \quad (44)$$

A variation on this theme involves using a reference sensitizer ( $S'$ ), to act as a triplet energy donor to transfer energy to another sensitizer viz.,



in the presence of oxygen and an oxidizable substrate. In the absence of absorption by  $S$ , of singlet state reaction by

S or S' and of singlet state sensitization and if reaction 23 is 100% efficient, then  $f_{\Delta}^T(S)$  can be obtained relative to  $f_{\Delta}^T(S')$  since

$$f_{\Delta}^T(S) = \frac{f_{\Delta}^T(S')P_T^{Q_2}(S')\phi_{ox}(S' + S)}{P_T^{Q_2}(S)\phi_{ox}(S')} \quad (45)$$

where  $\phi_{ox}(S' + S)$  is the quantum yield of oxidation of the substrate sensitized by the mixture of S' and S. Obviously here again any observable directly proportional to  $\phi_{ox}$  can also be used in Eq. (45).

Stevens *et al.*<sup>55</sup> have evolved a method for evaluating relative values of  $\phi_{\Delta}$  by the simultaneous excitation of two sensitizers one of which (S) does not react with or quench singlet oxygen whereas the other (S') does. If the absorbance at the exciting wavelength by S' and S are  $A_{S'}$  and  $A_S = A - A_{S'}$ , then the quantum yield of oxidation in terms of light absorbed by both S' and S is

$$\phi_{ox}(S + S') = p_A \left[ \frac{\phi_{\Delta}(S)A_S}{A} + \frac{\phi_{\Delta}(S')A_{S'}}{A} \right],$$

where  $\phi_{\Delta}(S)$  and  $\phi_{\Delta}(S')$  are the quantum yields of singlet oxygen production for S and S' respectively. The quantum yield of oxidation by S' alone at the same concentration of S' in the absence of sensitizer  $\phi_{ox}(S') = p_A\phi_{\Delta}(S')$ . N.B. S' = A, an oxidizable substrate which undergoes self-sensitization and substitution into the equation above gives upon rearrangement

$$\frac{\phi_{ox}(S + S')A}{\phi_{ox}(S')A_{S'}} - 1 = \frac{\phi_{\Delta}(S)}{\phi_{\Delta}(S')} \left[ \frac{A}{A_{S'}} - 1 \right] \quad (46)$$

and thus the relative values of  $\phi_{\Delta}$  have been obtained from plots of  $\phi_{ox}(S + S') \frac{A}{\phi_{ox}(S')A_{S'}} - 1$  versus  $\frac{A}{A_{S'}} - 1$ . Equation (46) needs to be modified if energy transfer between S and S' occurs.<sup>55</sup>

Carre *et al.*<sup>56</sup> have compared the rate of disappearance of DPBF as a reference substrate A' when sensitized with Methylene Blue as a reference sensitizer in the presence and absence of several dyes A which both quench and react with  ${}^1O_2^*$ . When absorption is only by S' in the presence of A and A' Eq. (14) becomes

$$-\frac{d[A']}{dt} = \frac{I_a\phi_{\Delta}(S')k_{A'}[A']}{k_d + k_{A'}[A'] + (k_q^A + k_r^A)[A]}$$

since  $k_r^A = k_{A'}$  for DPBF. When both S' and the dye absorbs at the exciting wavelength i.e. A = S, Eq. (14) gives

$$-\frac{d[A']}{dt} = \frac{\{I_a(S')\phi_{\Delta}(S') + I_a(S)\phi_{\Delta}(S)\}k_{A'}[A']}{k_d + k_{A'}[A'] + (k_q^S + k_r^S)[S]} \quad (47)$$

Carre *et al.*<sup>56</sup> used integrated forms of Eq. (47) to give  $\phi_{\Delta}(S)$  relative to  $\phi_{\Delta}(S')$  and by assuming  $\phi_{\Delta} = \phi_T$  (i.e. that Eq. (42) holds with  $f_{\Delta}^T = 1$ ) they report  $\phi_{\Delta}$  as values for  $\phi_{\Delta}$ .

#### 4.1.2. Pulsed Studies of Acceptor Disappearance

When a sensitizer S is excited by a laser pulse in the presence of oxygen and a reactive substrate A (such as DPBF), the amount of DPBF consumed is proportional to  $\phi_{\Delta}(S)$ . Thus if the change (reduction) in absorbance  $\Delta A_A$  caused by the laser pulse is measured for excitation of optically matched solutions of S and S', then it follows that since  $\phi_{ox}(S)$  is proportional to  $\Delta A_A(S)$  substitution in Eq. (43) gives another form of that equation; i.e.,

$$\frac{\phi_{\Delta}(S)}{\phi_{\Delta}(S')} = \frac{\Delta A_A(S)}{\Delta A_A(S')} \quad (43)$$

The decrease in absorbance of a reactive substrate following excitation by a laser pulse measured at an analyzing wavelength where only A absorbs is given by

$$\Delta A_A = [{}^1O_2^*]^o p_A \epsilon_A l$$

where  $[{}^1O_2^*]^o$  represents the concentration of singlet oxygen generated by the laser pulse,  $\epsilon_A$  is the extinction coefficient of A and  $l$  the path length. The amount of triplet state of the sensitizer produced by an identical pulse  $[{}^3S^*]^o$  can be measured by detecting the change in absorption due to triplet state absorption  $\Delta A_T$ . Thus

$$\Delta A_T = [{}^3S^*]^o \epsilon_T l$$

where  $\epsilon_T$  is the triplet state extinction coefficient at an analyzing wavelength where the ground state of the sensitizer does not absorb. The number of singlet oxygen molecules found per triplet state formed  $n_{\Delta}$  is given by

$$n_{\Delta} = \frac{\phi_{\Delta}}{\phi_T^{Q_2}} = \frac{\phi_T^{Q_2}P_T^{Q_2}f_{\Delta}^T + P_S^{Q_2}f_{\Delta}^S}{\phi_T^{Q_2}} = \frac{[{}^1O_2^*]^o}{[{}^3S^*]^o} = \frac{\Delta A_A \epsilon_A}{\Delta A_T p_A \epsilon_A} \quad (48)$$

When analysis is made at a wavelength where both the ground state and triplet state absorb,  $\epsilon_T$  in Eqs. (48) and (49) should be replaced by  $\Delta \epsilon_T = \epsilon_T - \epsilon_G$ . Equation (48) has various limits e.g.

$$n_{\Delta} = n_{\Delta}^T = f_{\Delta}^T$$

when  $P_T^{Q_2} = 1$  from type T and type TC sensitizers,

$$n_{\Delta} = n_{\Delta}^{ST} = f_{\Delta}^T + \frac{f_{\Delta}^S}{f_T^{Q_2}}$$

when  $P_T^{Q_2} = 1$  and  $P_S^{Q_2} = 1$ , for type ST sensitizers, and

$$n_{\Delta} = n_{\Delta}^{ST} = f_{\Delta}^T + f_{\Delta}^S$$

when  $P_T^{Q_2} = 1$ ,  $P_S^{Q_2} = 1$  and  $f_T^{Q_2} = 1$ . The maximum value of  $n_{\Delta}^{ST}$  is 2 when  $f_T^{Q_2} = P_S^{Q_2} = f_T^S = f_{\Delta}^T = f_{\Delta}^S = 1$  (see Ref. 57).

Chattopadhyay *et al.*<sup>58</sup> have reported an analogous method for measuring  $\phi_{\Delta}$  where two solutions are flashed under identical conditions with equal absorption by the

sensitizer in the presence of DPBF and oxygen on the one hand and by a triplet actinometer, AC, in the absence of oxygen and DPBF on the other. In the first case the change in absorbance of DPBF following excitation  $\Delta A_A$  is measured and in the second case the absorbance by the triplet state of the sensitizer  $A_T^{AC}$  is measured. Since  $I_a$  and the path length etc. are identical in the two experiments it follows that

$$\frac{\Delta A_A}{A_T^{AC}} = \frac{\epsilon_A \phi_A p_A}{\phi_T^{AC} \epsilon_T^{AC}}$$

which rearranges to give

$$\phi_A = \frac{\Delta A_A \phi_T^{AC} \epsilon_T^{AC}}{A_T^{AC} \epsilon_A p_A}. \quad (49)$$

Usually it is assumed that DPBF does not physically quench singlet oxygen and thus  $p_A \rightarrow 1$  as  $[A] \rightarrow \infty$ . It is also necessary that DPBF does not quench the sensitizer. The method needs to be treated with care. Thus Scaiano *et al.*<sup>59</sup> extrapolated their data to 'zero laser dose' to eliminate nonlinear effects due to the triplet state of benzophenone, the actinometer they used, absorbing at the laser wavelength. Due allowance also has to be made for any auto-oxidation due to DPBF absorbing the laser pulse and for the possibility of the excited sensitizer reacting with singlet oxygen.

In addition relative values of  $f_A^T$  have been obtained by subjecting optically matched cells at the laser excitation wavelength of one solution containing a sensitizer S and another containing a reference sensitizer S', to laser photolysis. In one case this procedure was applied in the presence of oxygen and DPBF and in the other in deaerated solution containing the addition of a high concentration of a triplet acceptor TA (e.g. 0.1 mol L<sup>-1</sup> 1-methylnaphthalene (1-MeNp) used to quench > 99% of sensitizer triplet states by energy transfer to give triplet 1-methylnaphthalene<sup>60</sup>). If  $A_T^T(S)$  and  $A_T^T(S')$  represent the absorbance observed for the triplet acceptor formed by energy transfer from <sup>3</sup>S and <sup>3</sup>S' respectively and  $\Delta A_A(S)$  and  $\Delta A_A(S')$  the measured change in absorbance by the reactive substrate A, then

$$\frac{f_A^T(S)}{f_A^T(S')} = \frac{\Delta A_A(S) A_T^T(S') P_T^O(S')}{\Delta A_A(S') A_T^T(S) P_T^O(S)}. \quad (50)$$

## 4.2. Photothermal Methods

A useful review of and general introduction to these methods is given by Braslavsky and Heihoff.<sup>61</sup>

### 4.2.1. Steady-State Photocalorimetric Methods

Photocalorimetric studies have been used to measure triplet quantum yields of sensitizers and overall reaction quantum yields involving singlet oxygen. It can be shown that heating rates of nonfluorescent sensitizer solutions

in the presence and absence of a singlet oxygen acceptor, if measured over short equal time intervals, are proportional to  $\Delta T$  and  $\Delta T_A$ , the temperature rises without and with the additive respectively. It is shown that

$$\frac{\Delta T - \Delta T_A}{\Delta T} = \frac{\phi_{ox} \Delta H_{ox}}{Nh\nu} \quad (51)$$

where  $\phi_{ox}$  is the quantum yield of the reaction with enthalpy change  $\Delta H_{ox}$ , N and h are Avogadro's and Planck's constants, and  $\nu$  is the frequency of the absorbed light. Olmsted<sup>62</sup> used this technique to show that  $\phi_{ox}$  for TPP (tetraphenylporphine) sensitized photo-oxidation of DMF, DPBF and TME (2,3-dimethyl-2-butene) in CCl<sub>4</sub>, at concentrations where  $\phi_{ox}$  is independent of concentration, are identical and equal to 0.88 ± 0.02. This implies  $\phi_T p_A$  for TPP in CCl<sub>4</sub> is > 0.88 and that  $\phi_A$  for all three acceptors is the same and most probably therefore equal to unity. In fact, Olmsted obtained  $\phi_{ox}$  for DPBF and TME in Freon equal to 1.00 ± 0.03 implying that  $\phi_T$ ,  $\phi_A$  and  $p_A$  all equal unity in this solvent.

### 4.2.2. Time Dependent Thermal Lensing

The fraction of heat dissipated slowly as <sup>1</sup>O<sub>2</sub>\* decays as measured in thermal lensing experiments (see also Section 3.2) is

$$\frac{\Delta U}{U_{tot}} = \frac{\phi_A <\nu_A>}{(\nu_l - \phi_F <\nu_F>) \quad (52)}$$

where  $<\nu_A>$  is the average frequency of emission of singlet oxygen,  $\nu_l$  is the frequency of the laser and  $\phi_F$  is the yield and  $<\nu_F>$  is the integrated average frequency of the sensitizer fluorescence in the aerated solution. Equation (52) has been used to determine absolute values of  $\phi_A$  from time dependent thermal lensing experiments.<sup>63,64</sup>

### 4.2.3. Laser Induced Photoacoustics

It is well known that when a solid or a liquid is irradiated with a modulated beam of light, the fraction of the light absorbed by the sample, converted into heat, causes a pressure wave at the surface. This photoacoustic wave can be detected (e.g. by a microphone) and used to obtain absorption spectra as in a photoacoustic spectrometer. When a laser excites an absorbing solution the first photoacoustic peak has an amplitude  $H$  given by

$$H = K \alpha I_a,$$

where  $I_a$  is the intensity of the light absorbed and  $K$  is a constant depending on the thermoelastic properties of the media as well as on instrumental parameters, geometry, etc. and  $\alpha$  is the fraction of the energy dissipated as heat within the time resolution of the experiment  $\tau_a$ . Energy balance requires<sup>65</sup>

$$\alpha = 1 - \frac{\phi_F^O <\nu_F>}{\nu_l} - \frac{\phi_A <\nu_A>}{\nu_l} \exp(-k_D \tau_a) \quad (53)$$

where  $k_D$  is the decay constant of the slowly decaying transient, ( $^1\text{O}_2^*$ ) in this case. Experimental measurements can be calibrated since dissipation of all of the energy in a time  $\tau \ll \tau_a$  gives  $\alpha = 1$ . For example, solutions of benzophenone containing a high concentration of potassium iodide can be used to give  $\alpha = 1$ .<sup>66</sup> In this way Eq. (53) has been used to measure  $\phi_\Delta$ .<sup>65</sup>

### 4.3. Luminescence Intensity Measurements

The quantum yield of phosphorescence of  $^1\text{O}_2^*$  is related to  $\phi_\Delta$  as follows

$$\phi_P^\Delta = \phi_\Delta f_P^\Delta = \frac{\phi_\Delta \tau_\Delta}{\tau_P^\Delta}, \quad (54)$$

where  $f_P^\Delta$  is the fraction of  $^1\text{O}_2^*$  formed which emits. For a discussion of the problems associated with the determination of absolute quantum yields of phosphorescence and radiative lifetimes of singlet oxygen see Ref. 68. In most solvents it is particularly difficult to measure  $\phi_P^\Delta$  because the values are very small (e.g. they are  $\sim 10^{-6}$  and  $\sim 10^{-4}$  in water and benzene, respectively). However for solvents in which there are no high energy vibrations (e.g. CS<sub>2</sub>, CCl<sub>4</sub> and ClCF<sub>2</sub>CCl<sub>2</sub>F), much higher yields are observed<sup>69</sup> (viz. 0.06, 0.09 and 0.15, respectively). The singlet oxygen lifetimes in these solvents are several milliseconds. If  $\tau_P^\Delta$ , the radiative lifetime were independent of solvent, relative measurements of phosphorescence intensities combined with known singlet oxygen lifetimes would give relative values for  $\phi_P^\Delta$ . However since the radiative process  $^1\Delta_g \leftarrow ^3\Sigma_g^-$  for the symmetrical molecule O<sub>2</sub> is highly forbidden,  $\tau_P^\Delta$  is highly solvent-dependent and estimates of  $\phi_P^\Delta$  and  $\tau_P^\Delta$  in the literature are often widely different. However relative measurements in the same solvent are directly proportional to  $\phi_\Delta$  and much use has been made of this as a probe for singlet oxygen.

For compounds where  $f_A^\Delta = 0$ , relative values of  $f_A^\Delta$  can be obtained from matched solutions by measurement of relative luminescence intensities at 1270 nm using the same solvent for S and S' extrapolated back to time  $t = 0$  ( $L_\Delta(S)_{t=0}$ ) and of the absorbance of the triplet state generated from identical laser pulses ( $A_T(S)$ ). The relationship used is:

$$\frac{f_A^\Delta(S)}{f_A^\Delta(S')} = \frac{L_\Delta(S)_{t=0} A_T(S') \epsilon_T(S) P_T^{Q_2}(S')}{L_\Delta(S')_{t=0} A_T(S) \epsilon_T(S') P_T^{Q_2}(S)}. \quad (55)$$

Relative measurements of singlet oxygen luminescence decay curves following pulse laser excitation of sensitizers can also be used to obtain relative  $\phi_\Delta$  values. Usually the luminescence intensities measured under identical conditions are extrapolated to time  $t = 0$  when

$$\frac{\phi_\Delta(S)}{\phi_\Delta(S')} = \frac{L_\Delta(S)_{t=0}}{L_\Delta(S')_{t=0}}. \quad (56)$$

Sometimes this ratio is extrapolated to zero laser intensity thus eliminating any possible nonlinear effects.<sup>37,58</sup>

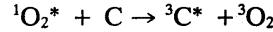
Often  $L_\Delta(S)_{t=0}$  is measured as a function of laser energy and the ratio of the slopes of linear plots of  $L_\Delta(S)_{t=0}$  versus  $I_L$  are used with Eq. (56) to give relative  $\phi_\Delta$  values. A comparison of values obtained by luminescence intensity measurement and time dependent thermal lensing is given in Ref. 67. Alternatively the ratio of the intensity of phosphorescence of singlet oxygen  $L_\Delta(S)$  observed from a sensitizer S relative to that observed from a suitable reference sensitizer S' ( $L_\Delta(S')$ ) excited and observed under identical continuous irradiation conditions is used in Eq. (56). Thus Eq. (56) applies to steady-state measurements provided neither S nor S' quenches singlet oxygen. It is a good practice to extrapolate such values to infinite dilution.<sup>58</sup>

If luminescence intensities are compared from different solvents the measured intensity  $L_\Delta$  must be corrected for differences in radiative probabilities by multiplying by  $\tau_P^\Delta$  and for differences in luminescence collection efficiencies which often depend on  $n^2$  (where  $n$  is the refractive index). Thus, corrected values  $L_\Delta^c$  have to be used in Eq. (56) where  $L_\Delta^c = L_\Delta n^2 \tau_P^\Delta$ .

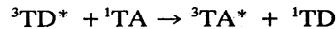
### 4.4. Triplet Energy Transfer and Singlet Oxygen Yields

#### 4.4.1. Using Triplet β-Carotene as a Probe

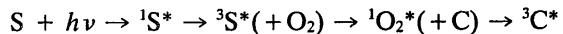
As mentioned earlier the sensitized production and decay of β-carotene arising from the process



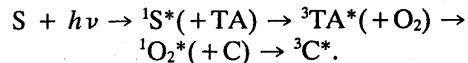
can be used for measuring singlet oxygen lifetimes<sup>45</sup> (see Paper I<sup>26</sup>). This reaction is very efficient and has a rate constant of  $1.2 \times 10^{10} \text{ L mol}^{-1} \text{ s}^{-1}$  in benzene solution, producing  $^3\text{C}^*$  which has a strong absorption band at  $\sim 520 \text{ nm}$ . The process of triplet energy transfer from a donor (TD) to an acceptor (TA) is also very efficient; i.e.,



and  $^3\text{TA}^*$  can act as a singlet oxygen sensitizer. Garner and Wilkinson<sup>70</sup> were the first to employ this process using a series of different energy acceptors to determine relative singlet oxygen yields by observing the different amounts of triplet β-carotene produced extrapolated to zero time. Matched solutions containing concentrations of reagents selected so that the following sequence of reactions could be observed were flashed,



and compared with



A full kinetic analysis is given in Ref. 70. It is sufficient to observe here that when S was xanthone dissolved

in benzene without addition of naphthalene as a triplet acceptor, the amount of absorbance by  ${}^3\text{C}^*$  at 520 nm extrapolated to zero time  $A_{\text{T}}^{\text{C}}(\text{S})$  was only 30% of that observed when the extra step of energy transfer to naphthalene occurred  $A_{\text{T}}^{\text{C}}(\text{TA})$ . After correcting for the fractions of  ${}^3\text{S}^*$  and  ${}^3\text{TA}^*$  intercepted by oxygen the ratio  $f_{\Delta}^{\text{T}}(\text{xanthone})/f_{\Delta}^{\text{T}}(\text{naphthalene})$  was shown to be  $\leq 0.55$ . The equality sign applies if the efficiency for energy transfer from triplet xanthone to give triplet naphthalene is 100%. When energy transfer is 100%

$$\frac{f_{\Delta}^{\text{T}}(\text{TA})}{\phi_{\Delta}(\text{S})} = \frac{A_{\text{T}}^{\text{C}}(\text{TA})P_{\text{T}}^{\text{O}_2}(\text{S})}{A_{\text{T}}^{\text{C}}(\text{S})P_{\text{T}}^{\text{O}_2}(\text{TA})}. \quad (57)$$

Comparison of  $A_{\text{T}}^{\text{C}}(\text{S})$  values for matched solutions of  $\text{S}$  and  $\text{S}'$  containing equal concentration of  $\beta$ -carotene gives a form of Eq. (43) viz

$$\frac{\phi_{\Delta}(\text{S})}{\phi_{\Delta}(\text{S}')}, \quad (43)$$

In this technique when different triplet energy acceptors  $\text{S}$  and  $\text{S}'$  are used with the same triplet donor, provided the efficiency of energy transfer is 100% in each case, then

$$\frac{f_{\Delta}^{\text{T}}(\text{S})}{f_{\Delta}^{\text{T}}(\text{S}')} = \frac{P_{\text{T}}^{\text{O}_2}(\text{S}')A_{\text{T}}^{\text{C}}(\text{S})}{P_{\text{T}}^{\text{O}_2}(\text{S})A_{\text{T}}^{\text{C}}(\text{S}')} \quad (58)$$

where  $A_{\text{T}}^{\text{C}}(\text{S})$  and  $A_{\text{T}}^{\text{C}}(\text{S}')$  are the observed amount of absorbance by  ${}^3\text{C}^*$  when  $\text{TA} = \text{S}$  and  $\text{S}'$  respectively. A similar technique using  $\beta$ -carotene as a probe was used in pulse radiolysis experiments to measure  $f_{\Delta}^{\text{T}}$  for substrates relative to that for benzophenone.<sup>71</sup> In Ref. 71 the relative amounts of triplet states formed in the absence of  $\text{O}_2$  and  $\beta$ -carotene were calculated by measuring the absorbance by the sensitizer triplets  $A_{\text{T}}(\text{S})$  and  $A_{\text{T}}(\text{S}')$  and using known extinction coefficients ( $\epsilon_{\text{T}}$ ) to give

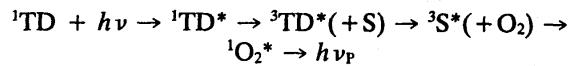
$$\frac{f_{\Delta}^{\text{T}}(\text{S})}{f_{\Delta}^{\text{T}}(\text{S}')} = \frac{A_{\text{T}}^{\text{C}}(\text{S})\epsilon_{\text{T}}(\text{S})P_{\text{T}}^{\text{O}_2}(\text{S}')A_{\text{T}}(\text{S}')}{A_{\text{T}}^{\text{C}}(\text{S}')\epsilon_{\text{T}}(\text{S}')P_{\text{T}}^{\text{O}_2}(\text{S})A_{\text{T}}(\text{S})}, \quad (59)$$

where  $A_{\text{T}}^{\text{C}}$  is the absorption by  ${}^3\text{C}^*$  observed at 540 nm due to energy transfer from singlet oxygen, extrapolated to zero time.

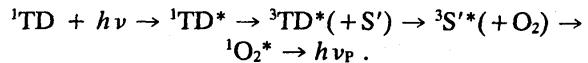
#### 4.4.2. Using Luminescence Measurements

With the development of singlet oxygen luminescence decay measurements a simpler technique is to measure the decay of singlet oxygen luminescence and the intensity extrapolated to time  $t = 0$  ( $L_{\Delta}(\text{S}),_{t=0}$ ) following laser excitation of matched solutions in which 100% efficient energy transfer takes place. Using aromatic ketones, for which  $P_{\text{S}}^{\text{O}_2} = 0$  due to their short singlet state lifetimes as triplet donors (TD) relative values of  $f_{\Delta}^{\text{T}}$  can be obtained

from  $L_{\Delta}$  values measured under identical conditions. The reaction sequence is as follows



compared with



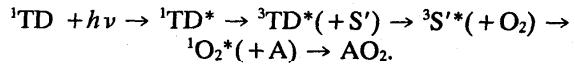
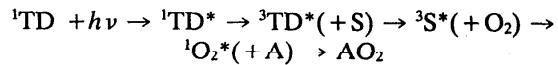
In the absence of absorption of exciting light by  $\text{S}$  and  $\text{S}'$  and when the efficiencies of energy transfer to the sensitizers are both unity, then relative values of  $f_{\Delta}^{\text{T}}$  are given by

$$\frac{f_{\Delta}^{\text{T}}(\text{S})}{f_{\Delta}^{\text{T}}(\text{S}')} = \frac{L_{\Delta}(\text{S}),_{t=0}P_{\text{T}}^{\text{O}_2}(\text{S}')}{L_{\Delta}(\text{S}'),_{t=0}P_{\text{T}}^{\text{O}_2}(\text{S})}. \quad (60)$$

If the transfer efficiencies (i.e. the fractional quenching of the triplet state of the  ${}^3\text{TD}^*$  by  $\text{S}$  and  $\text{S}'$ ) are known to be less than unity, due allowance can be made. Gorman *et al.*<sup>37</sup> introduced this technique and suggest using naphthalene as the standard of choice in a variety of situations. See also Section 4.1.2.

#### 4.4.3. Using Pulsed Studies of Acceptor Disappearance

An analogous method for measuring relative  $f_{\Delta}^{\text{T}}$  values makes use of a reactive reactant such as DPBF as a probe for singlet oxygen production. The reactive sequence is similar:



In the absence of absorption of the exciting light by  $\text{A}$ ,  $\text{S}$  or  $\text{S}'$  and when the efficiency of energy transfer is unity then under identical matched conditions

$$\frac{f_{\Delta}^{\text{T}}(\text{S})}{f_{\Delta}^{\text{T}}(\text{S}')} = \frac{\Delta A_{\text{A}}(\text{S})P_{\text{T}}^{\text{O}_2}(\text{S}')}{\Delta A_{\text{A}}(\text{S}'),_{t=0}P_{\text{T}}^{\text{O}_2}(\text{S})}, \quad (61)$$

where  $\Delta A_{\text{A}}$  is the decrease in the absorbance of  $\text{A}$  due to reaction with singlet oxygen. See also Section 4.1.1.

A variation on this theme uses a ketone with  $P_{\text{S}}^{\text{O}_2} = 0$  as both triplet donor and as an actinometer by measuring the change in absorbance due to the triplet donor absorption at time  $t = 0$ , in which case

$$f_{\Delta}^{\text{T}}(\text{S}) = \frac{\Delta A_{\text{A}}(\text{TD} + \text{S})P_{\text{T}}^{\text{O}_2}(\text{TD})}{\Delta A_{\text{A}}(\text{TD})\epsilon_{\text{A}}P_{\text{T}}^{\text{O}_2}(\text{S})}. \quad (62)$$

Again it is necessary for the energy transfer from the triplet donor to be 100% efficient.

## 5. Quantum Yields of Singlet Oxygen Production – Comments on the Tables

### 5.1. Contents of Tables 1–3

Quantitative data for photosensitized singlet oxygen production are given in three tables containing 1,600 separate entries for 750 chemical species. Tables 1–3 follow Sec. 8. The main table (Table 1) contains data for 316 compounds which convert molecular oxygen into singlet oxygen via their excited triplet and/or singlet states with varying efficiencies. Porphyrins and related species have been collected into Table 2. An additional table (Table 3) has been provided for dyes, polymers and some other species which, although they are ill-defined, are of interest for various biomedical, environmental, and industrial applications. The arrangement of the tables is alphabetic by the chemical names of the photosensitizers. Common names have been used for a few compounds; otherwise, systematic names have been entered. Inverted names have been used in most cases so that substituted acetophenones, anthracenes, fluoresceins, etc. are grouped. An index of chemical names and synonyms and a formula index follow the tables (Secs. 10 and 11) and refer to the entry numbers in Tables 1–3.

Oxygen concentrations are given when they have been reported or else the column headed  $[O_2]$  contains 'air' or ' $O_2$ ' to indicate that the solution was air- or oxygen-saturated. The *Solvent* column gives the solvent or mixture of solvents with the proportions (volume:volume) and the pH or pD, if reported. Heterogeneous systems are identified, (e.g. as micellar (mic)), and the surfactant present is given in the *Comments*. Data for each photosensitizer are grouped by solvent and listed in reverse chronological order.

Values in the quantum yield column may be tagged with a superscript T to denote quantum yields representing 100% quenching of  $T_1$ , or ST representing 100% quenching of both  $S_1$  and  $T_1$ . Most of the quantum yields tagged T are for type T sensitizers which have  $P_{S^2}^{O_2} = 0$ . However limiting yields of singlet oxygen production from  $T_1$  have been obtained in other cases by adjusting oxygen concentrations or by correcting for oxygen quenching of the sensitizer singlet states. Evaluation of  $P_{S^2}^{O_2}$  and  $P_{T^2}^{O_2}$  has enabled the determination of  $\phi_A^T$  and  $\phi_A^{ST}$  (see Sec. 4). When  $P_{T^2}^{O_2}$  has been measured for type T sensitizers,  $f_A^T$  is known through  $\phi_T(S)$  and Eqs. (41) and (42). If values of  $\phi_T(S)$  have been used to calculate  $f_A^T$  from  $\phi_A$  (or the reverse) they are given in the comments. Data for the  $f_A^S$  column, and the column labeled  $\Sigma f$  ( $f_A^T + f_A^S$ ) or  $n_A$  (the number of singlet oxygen molecules produced per triplet state formed) are sparse; see Sec. 4.1.2 for limits on  $n_A$  for type T, type TC and type ST sensitizers.

Codes in the *Method* column combine symbols (see Sec. 6) representing the excitation technique, the measurement technique, and the numbers of the equations given above which have been used for analyzing the data. If two measurement techniques or equations were used

the symbols are combined. For example, PL/LI-56,42 represents the pulsed-laser luminescence-intensity technique and refers to both Eqs. (56) and (42) to obtain values for  $\phi_A$  and  $f_A^T$ .

Some details of the determination are given in the *Comments* column. Abbreviations and symbols are listed in Sec. 6 for chemical species which have been used as reference sensitizer (S'), triplet donor (TD), triplet acceptor (TA), actinometer (AC), and acceptor of singlet oxygen (A). Values for  $\phi_A$  and  $f_A^T$  of the reference sensitizer which have been used to obtain the tabulated data are given. Quantum yields and extinction coefficients for the triplet states have been included when their values have been used for obtaining the singlet oxygen yields. Temperature is included in the *Comment* if it has been reported to be outside the range of about 20–25°C.

Codes in the *Reference* column are from the Radiation Chemistry Data Center Bibliographic Database. The first two characters of the reference code identify the year of publication. The complete references to the tables are listed in Sec. 9 which follows the tables.

### 5.2. Relative Measurements and Standard Values

Often  $f_A^T$  or  $\phi_A$  have been determined relative to the known value for another sensitizer so that the values depend on the standard values chosen for the reference sensitizer. It would be desirable to obtain the best possible values for  $f_A^T$  and  $\phi_A$  for the reference sensitizers based on the measured values which have been reported. Unfortunately  $f_A^T$  for each sensitizer depends on the solvent (on pH etc.) and so it is necessary to treat the values for each solvent separately. For sensitizers other than type T, values of  $\phi_A$  depend on the concentration of oxygen even when  $P_{T^2}^{O_2} = 1$ . For those classes of sensitizer (e.g. type ST and TC) we must therefore treat separately the values for each solvent saturated with air and oxygen, respectively.

Values reported as ratios with respect to the value for a reference sensitizer (e.g.  $f_A^T(S)/f_A^T(S') = R_f(S,S')$  or  $\phi_A(S)/\phi_A(S') = R_\phi(S,S')$ ) are often of greater accuracy than values obtained by methods used to measure  $f_A^T$  and  $\phi_A$  which do not give a ratio but may depend on other photophysical parameters (e.g.  $\phi_T$ ,  $\epsilon_T$  or  $\Delta\epsilon_T$ ) or relative or absolute values of  $\Delta A$ . Although the time-dependent thermal lensing and photo-acoustic methods, in principle, only depend on the standard used as a 100% heat producer to give  $\phi_A$ , values of  $\phi_T$  are needed, as in other methods, to convert  $\phi_A$  to  $f_A^T$  in the case of type T sensitizers. It has to be recognised that no accurate set of  $\phi_T$  values, however, is available. For example, the  $\phi_T$  in benzene for the important reference sensitizer acridine (Ac) is given in the literature as 0.73<sup>72</sup> and 1.0<sup>73</sup>. We have chosen to use the average value of 0.86 for  $\phi_T$  of Ac in benzene in Table 1.

Thus we have the situation where many values of  $\phi_A$  and  $f_A^T$  may be connected through ratios and errors of at least 10% are expected; inspection of the tables shows that agreement is often much worse than this. We have

therefore carried out an iterative averaging process to obtain a limited self-consistent set of average values. Similar procedures used to examine rate constants for reactions of singlet oxygen<sup>74</sup> and extinction coefficients for triplet-triplet absorption<sup>75</sup> have been described. Full details of the exact procedure used here are given in Appendix 2. The procedure gives self-consistent averages for  $f_A^T$  and a mutually self-consistent set of average values for  $\phi_A$ , where  $\phi_A^T$  is related to  $f_A^T$  through  $\phi_T$ . These values are given in Table A.2.1 (see Appendix 2).

Figure 4 shows the interconnections for the relative values of  $f_A^T$  in benzene, the solvent with the most interdependencies. Figure 4 demonstrates that the crucial compounds, the values for which are critical, are benzophenone (BP), acridine (Ac) and naphthalene (Np). In the case of BP, where  $\phi_T = 1$  and  $f_A^T = \phi_A$ , the ratio  $R_f$  (Np, BP) has been indicated to be 1.9 in several careful studies.<sup>37,70,71,76,77</sup> The global averages obtained for  $f_A^T$  of Np and BP in benzene (Table A.2.1) are 0.618 and 0.346, respectively, in the ratio 1.8. The values of 0.29 for BP and 0.55 for Np in benzene have been most often used

in the literature as standards. However the mathematical procedure has directed us to the higher value for BP and consequently, a higher value for Np. The value of 0.35 has been selected as the standard value for  $\phi_A$  and  $f_A^T$  of BP in benzene (see the following table). The global averages for  $f_A^T(\text{Ac}) = 0.99$  and  $\phi_A(\text{Ac}) = 0.83$  are in good agreement with recent papers<sup>67,78,79</sup> which have preferred  $\phi_A = 0.84$  as the standard reference value for acridine.

Selected reference values for  $\phi_A$  and  $f_A^T$ .

| No. <sup>a</sup> | S     | Solvent                       | [O <sub>2</sub> ] | $\phi_A$ | $f_A^T$ |
|------------------|-------|-------------------------------|-------------------|----------|---------|
| 1.1              | 2-ACN | C <sub>6</sub> H <sub>6</sub> |                   | 0.71     | 0.81    |
| 1.7              | Ac    | C <sub>6</sub> H <sub>6</sub> |                   | 0.83     | 0.99    |
| 1.88             | BP    | C <sub>6</sub> H <sub>6</sub> |                   | 0.35     | 0.35    |
| 1.169            | RB    | MeOH                          |                   | 0.80     |         |
| 1.169            | RB    | H <sub>2</sub> O              |                   | 0.76     |         |
| 1.220            | Np    | C <sub>6</sub> H <sub>6</sub> |                   |          | 0.62    |
| 1.239            | Pz    | C <sub>6</sub> H <sub>6</sub> |                   | 0.88     | 1.00    |
| 2.136            | TPP   | CCl <sub>4</sub>              | air               | 0.62     |         |

<sup>a</sup>Entry numbers in Tables 1 and 2.

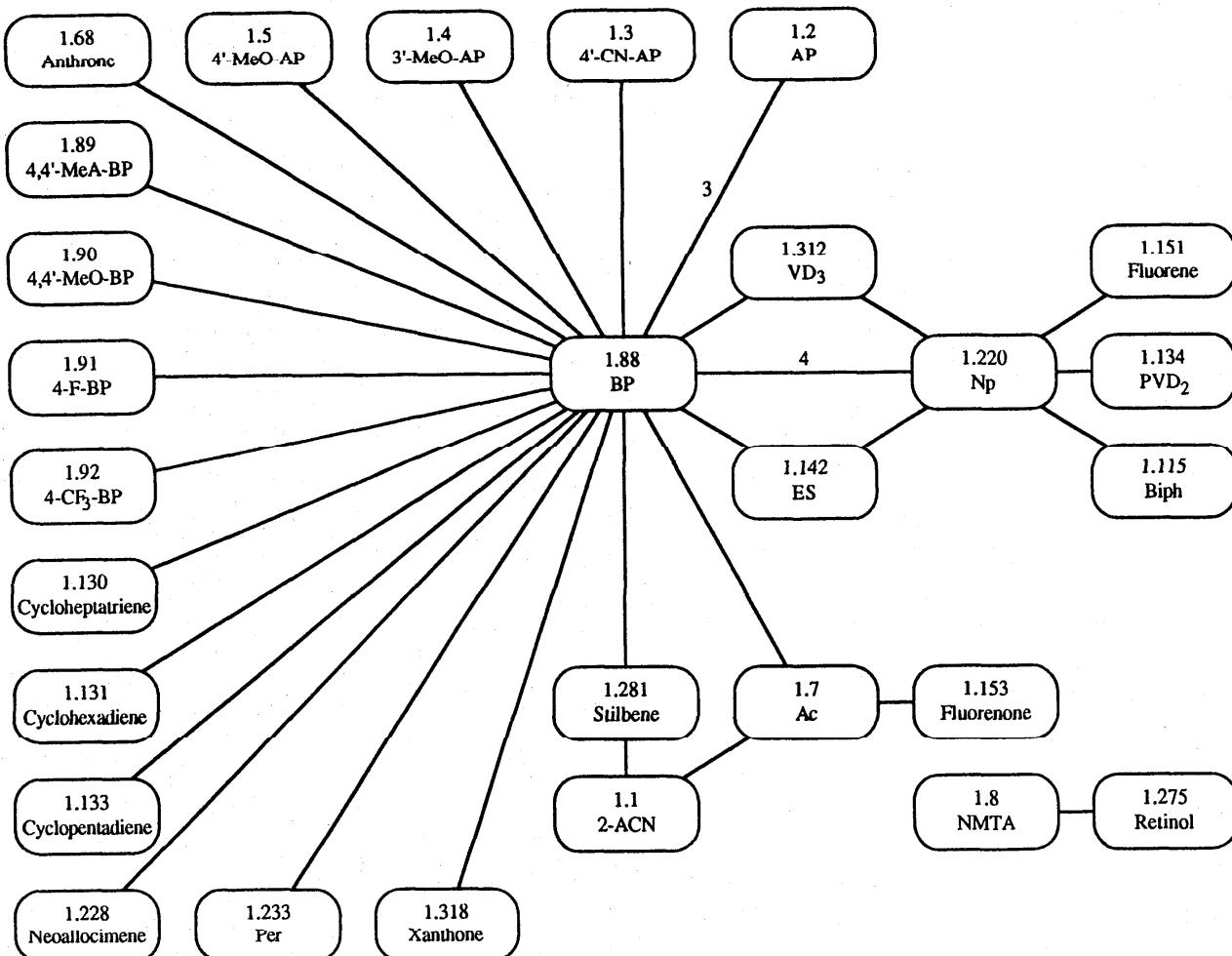


FIG. 4. Diagram showing connections between relative  $f_A^T$  measurements for photosensitizers in benzene. Entry numbers in Table 1 are given. Three ratios for acetophenone-benzophenone (AP-BP) and four for benzophenone-naphthalene (BP-Np) have been measured.

Whenever the average values given in Table A.2.1 differ by more than 10% from the reference values of  $S'$  used to calculate either  $f_A^T$  or  $\phi_\Delta$  from  $R_f(S, S')$  or  $R_\phi(S, S')$  we have recalculated those values. The table on p. 127 lists reference values derived from the global averaging process which have been used for recalculations. The recalculated values have been marked with an asterisk and listed in Tables 1-3 along with the reported data. We have also recalculated some values of  $\phi_\Delta$  relative to  $S' =$  hematoporphyrin (HP) in  $\text{CH}_3\text{OD}$  (e.g. see entry 1.245) where a recent paper identified in the entry has provided a value for  $\phi_\Delta(\text{HP})$  in  $\text{CH}_3\text{OD}$ .

In some cases only ratios of  $\phi_\Delta$  have been reported. We have converted reported ratios into absolute values by using the averages from Table A.2.1 when available, or using apparently accepted standards from the literature, or using a standard value inferred from other reported data. Footnote b in the tables identifies reference values used in this work to calculate absolute values from reported ratios. Many authors have used  $\phi_\Delta = 0.76$  or 0.75 for Rose Bengal (RB) as the reference value in a variety of solvents. The values obtained for water and methanol in the averaging procedure (Appendix 2) are 0.76 and 0.80, respectively. We have used  $\phi_\Delta(\text{RB}) = 0.76$  to calculate values for the  $\phi_\Delta$  column for data which have been quoted only as ratios in water, and  $\phi_\Delta(\text{RB}) = 0.80$  for data in ethanol, methanol, acetonitrile, acetone, and methylene chloride.

Other values used in this work to convert ratios to absolute values of  $\phi_\Delta(S)$  are 0.50 for methylene blue ( $\text{MB}^+$ ) in ethanol, 0.77 for mesoporphyrin dimethyl ester (MPDME) in chloroform, 0.4 for HP in water, 0.6 for HP in dimethylformamide or dioxane, and 0.3, 0.4, and 0.5 for riboflavin (RF) in  $\text{D}_2\text{O}$ , methanol and  $\text{H}_2\text{O}/\text{EtOH}$  (1:1), respectively.

The use of  $\phi_\Delta = 1$  for PdMPDME as a reference sensitizer has been justified (see entry 2.183). The same result has been obtained by the use of  $\phi_\Delta = 1$  for both PdMPDME and PdOEP (palladium octaethylporphine) for calculating absolute values for octaethylporphine (OEP) and ZnOEP (entries 2.73 and 2.83), therefore  $\phi_\Delta = 1$  has also been used for PdOEP to convert ratios to absolute values. No similar relationship was found for values relative to GaTPP (gallium tetraphenylporphine) in carbon tetrachloride so data involving that sensitizer are only available as ratios. In those cases the ratios are given in the *Comments* column. Ratios also remain for a group of platinum and palladium complexes (see entry 3.34 and subsequent entries in Table 3). Likewise, there are a number of metallated dyes (cf. entry 3.85 and following entries) for which there is no value in the  $\phi_\Delta$  column since only relative yields have been reported.

## 6. List of Abbreviations and Symbols

### Excitation Methods

|    |                             |
|----|-----------------------------|
| CL | continuous laser photolysis |
| CP | continuous photolysis       |
| MP | modulated photolysis        |

|                            |   |
|----------------------------|---|
| PL                         | pulsed laser photolysis   |
| PR                         | pulsed radiolysis   |
| <i>Measurement Methods</i> |   |
| Ac                         | substrate consumption under steady-state conditions                     |
| ACt                        | actinometer triplet absorbance at end-of-pulse                          |
| Ad                         | time resolved substrate disappearance                                   |
| $\beta_{\text{Cb}}$        | triplet beta-carotene buildup as a probe for singlet oxygen production  |
| Hp                         | heat produced from singlet oxygen                                       |
| LI                         | luminescence intensity at end-of-pulse or under steady-state conditions |
| Oc                         | oxygen consumption under steady-state conditions                        |
| Pa                         | product appearance under steady-state conditions                        |
| St                         | sensitizer triplet absorbance at end-of-pulse                           |
| TAt                        | triplet acceptor absorbance at end-of-pulse                             |
| TDt                        | triplet donor absorbance at end-of-pulse                                |
| Tr                         | temperature rise  |

### Other Symbols

|                     |  |
|---------------------|--|
| $\Delta A_A$        | change in absorption due to acceptor A                                       |
| $\Delta A_T$        | change in absorption due to triplet state                                    |
| A                   | substrate (singlet oxygen acceptor)  |
| A'                  | reference substrate  |
| AC                  | triplet actinometer  |
| $\beta_A$           | $k_A/k_A$  |
| $E_\Delta$          | energy of $\text{O}_2 (^1\Delta_g)$ above the ground state                   |
| $\Delta \epsilon_T$ | difference of extinction coefficients of triplet and ground state absorption |
| $\epsilon_T$        | extinction coefficient of triplet state absorption                           |
| F                   | fluorescence intensity of sensitizer   |
| $F^\circ$           | fluorescence intensity of sensitizer in presence of oxygen                   |
| $f_A^S$             | fraction of $S_1$ quenched by $\text{O}_2$ which gives singlet oxygen        |
| $f_A^T$             | fraction of $T_1$ quenched by $\text{O}_2$ which gives singlet oxygen        |
| $\Sigma f$          | $f_A^S + f_A^T$  |
| $f_A^S$             | fraction of singlet oxygen which emits                                       |
| $f_A^A$             | fraction of ${}^1\text{O}_2^*$ quenched by A which reacts                    |
| $f_{\text{O}_2}^S$  | fraction of $S_1$ quenched by $\text{O}_2$ which gives $T_1$                 |
| G                   | radiation yield, molecules per 100 eV  |
| $k_d$               | first-order decay rate of singlet oxygen in solvent                          |
| $k_\Delta$          | first-order decay rate of singlet oxygen for $[S] \rightarrow 0$             |
| $k_{\Delta P}$      | first-order radiative decay rate of singlet oxygen                           |
| $k_{\Delta d}$      | first-order radiationless decay rate of singlet oxygen                       |

|                              |   |                  |   |
|------------------------------|---|------------------|---|
| $k_A$                        | rate constant for reaction of singlet oxygen with substrate                   | BDX              | Benzo[1,2,3- <i>kl</i> :4,5,6- <i>k'l'</i> ]dixanthene                                |
| $k_q^A$                      | rate constant for physical quenching of A                                     | Biph             | Biphenyl  |
| $k_r^A$                      | rate constant for chemical reaction of A                                      | BP               | Benzophenone  |
| $k_s$                        | rate constant for reaction of singlet oxygen with sensitizer                  | BRH <sub>2</sub> | Bilirubin   |
| $K_{SV}$                     | Stern-Volmer constant for singlet quenching by O <sub>2</sub>                 | BR <sup>2-</sup> | Bilirubin dianion   |
| $L_\Delta$                   | luminescence intensity due to singlet oxygen                                  | BXP              | Benoxyprofen  |
| $\lambda_{exc}$              | wavelength of excitation  | Car              | $\beta$ -Carotene (also $\beta$ -C)   |
| $n_\Delta$                   | number of singlet oxygen molecules found per triplet state formed             | Cd(II) Dye I     | Cadmium(II) 1-(2-hydroxyphenylazo)-2-naphtholate                                      |
| ${}^1\text{O}_2^*$           | the first excited singlet state of molecular oxygen                           | Chl a            | Chlorophyll a   |
| P                            | product from substrate  | CQ               | Camphoroquinone   |
| $p_A$                        | fraction of substrate which reacts  | CZ               | Chlorpromazine  |
| $P_S^{Q_2}$                  | proportion of S <sub>1</sub> quenched by O <sub>2</sub>                       | DCA              | 9,10-Dicyanoanthracene  |
| $P_T^{Q_2}$                  | proportion of T <sub>1</sub> quenched by O <sub>2</sub>                       | DMA              | 9,10-Dimethylanthracene   |
| $\phi_\Delta$                | quantum yield of singlet oxygen formation                                     | 4,7-DMAPs        | 4,7-Dimethylallopsoralen  |
| $\phi_{et}$                  | quantum yield for energy transfer   | DMBA             | 9,10-Dimethylbenz[a]anthracene  |
| $\phi_{ox}$                  | quantum yield of oxidation of substrate                                       | DMDPA            | 1,4-Dimethoxy-9,10-diphenylanthracene   |
| $\phi_F$                     | quantum yield of fluorescence   | 2,5-DMF          | 2,5-Dimethylfuran   |
| $\phi_F^{Q_2}$               | quantum yield of fluorescence in the presence of O <sub>2</sub>               | DMTBP            | 4,4'-Dimethoxythiobenzophenone  |
| $\phi_P^A$                   | quantum yield of phosphorescence of singlet oxygen                            | DNT              | 1,8-Dinaphthalene thiophene (Diacenaph-tho[1,2- <i>b</i> :1',2'- <i>d</i> ]thiophene) |
| $\phi_T$                     | quantum yield of triplet formation (inter-system crossing yield)              | DOPA             | 3-(3,4-Dihydroxyphenyl)alanine  |
| $\phi_T^{Q_2}$               | quantum yield of triplet formation in the presence of O <sub>2</sub>          | DPA              | 9,10-Diphenylanthracene   |
| S                            | sensitizer  | DPB              | 1,4-Diphenyl-1,3-butadiene  |
| ${}^3\text{S}^*$             | sensitizer triplet  | DPBF             | 1,3-Diphenylisobenzofuran   |
| S'                           | reference sensitizer  | DPF              | 2,5-Diphenylfuran   |
| TA                           | triplet acceptor  | DPH              | 1,6-Diphenyl-1,3,5-hexatriene   |
| TD                           | triplet donor   | DPO              | 1,8-Diphenyl-1,3,5,7-octatetraene   |
| $\tau_r$                     | radiative lifetime  | DTBF             | 2,5-Di- <i>tert</i> -butylfuran   |
| $\tau_\Delta$                | lifetime of singlet oxygen  | Eos              | Eosin (Tetrabromofluorescein)   |
| $\tau_P^A$                   | radiative lifetime of singlet oxygen  | Ery              | Erythrosin (Tetraiodofluorescein)   |
| $\langle \nu_F \rangle$      | integrated average frequency of sensitizer fluorescence in presence of oxygen | ES               | Ergosterol  |
| $\langle \nu_\Delta \rangle$ | integrated average frequency of emission of singlet oxygen                    | FFA              | Furfuryl alcohol  |

|  |  |                                       |  |
|--|--|---------------------------------------|--|
| <i>Reference Sensitizers, Acceptors, Triplet acceptors, Triplet actinometers</i> |  |                                       |  |
| Ac   | Acridine   | MPDEE                                 | Mesoporphyrin diethyl ester                        |
| 2-ACN  | 2-Acetonaphthone                                     | MPDME                                 | Mesoporphyrin dimethyl ester                       |
| ADC  | Anthra[1,9- <i>bc</i> :4,10- <i>b'c'</i> ]dichromene | NMTA                                  | 10-Methyl-9-acridinethione                         |
| ADPA   | 9,10-Anthracenedipropionate ion                      | Np                                    | Naphthalene  |
| AIPCS  | Aluminum(III) sulfophthalocyanine                    | PdTPP                                 | Palladium(II) tetraphenylporphyrin                 |
| An   | Anthracene   | PdTPPS <sup>4-</sup>                  | Palladium(II) tetrakis(4-sulfonatophenyl)porphyrin |
| Ang  | Angelicin  | Per                                   | Perylene   |
| AnS  | Anthracenesulfonate ion                              | Ph a                                  | Pheophytin a                                       |
| AP   | Acetophenone   | PP                                    | Protoporphyrin                                     |
| AQ   | 9,10-Anthraquinone                                   | PPDME                                 | Protoporphyrin dimethyl ester                      |
| ATU  | Allylthiourea  | PrPor                                 | 2,7,12,17-Tetrapropylporphycene                    |
| BChl a   | Bacteriochlorophyll a                                | Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> | Platinum(II) diazido(2,2'-bipyridine)              |

|                                    |   |              |  |
|------------------------------------|---|--------------|--|
| Pt(phen)<br>(BCAT)                 | Platinum(II) (1,10-phenanthroline)( <i>tert</i> -butylcatechol) | py           | Pyridine   |
| Pt(phen)<br>(dhn)                  | Platinum(II) (1,10-phenanthroline)(2,3-naphthalenediol)         | SDS          | Sodium dodecylsulfate  |
| Py                                 | Pyrene  | THF          | Tetrahydrofuran  |
| Pz                                 | Phenazine   | Triton X-100 | Polyoxyethylene(10) 4-(1,1,3,3-tetramethylbutyl)phenyl ether |
| RB                                 | Rose Bengal (Tetrachlorotetraiodofluorescein)                   | ves          | vesicles   |
| RBEE                               | Rose Bengal ethyl ester   |              |  |
| Ret                                | ( <i>all-E</i> )-Retinal  |              |  |
| RF                                 | Riboflavin  |              |  |
| RNO                                | <i>N,N</i> -Dimethyl-4-nitrosoaniline                           |              |  |
| Rub                                | Rubrene (5,6,11,12-Tetraphenylnaphthacene)                      |              |  |
| TEMP-4-OH                          | 2,2,6,6-Tetramethylpiperidin-4-ol                               |              |  |
| Tetr                               | Tetracene   |              |  |
| T(m-HOP)P                          | Tetra(3-hydroxyphenyl)porphyrin                                 |              |  |
| T(p-HOP)P                          | Tetra(4-hydroxyphenyl)porphyrin                                 |              |  |
| TME                                | 2,3-Dimethyl-2-butene (Tetramethylethylene)                     |              |  |
| H <sub>2</sub> TMpyP <sup>4+</sup> | Tetra(4- <i>N</i> -methylpyridyl)porphyrin                      |              |  |
| TPBC                               | Tetraphenylbacteriochlorin                                      |              |  |
| TPCP                               | Tetraphenylcyclopentadienone                                    |              |  |
| TPP                                | Tetraphenylporphyrin  |              |  |
| H <sub>2</sub> TPPS <sup>4-</sup>  | Tetra(4-sulfonatophenyl)porphyrin                               |              |  |
| TrpH                               | Tryptophan  |              |  |
| UP                                 | Uroporphyrin I  |              |  |
| ZnTPP                              | Zinc(II) tetraphenylporphyrin                                   |              |  |
| Zn(II) Dye II                      | Zinc(II) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate      |              |  |
| Zn(II) Dye III                     | Zinc(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate      |              |  |

*Medium components*

|                   |                                      |
|-------------------|--------------------------------------|
| AOT               | Di(2-ethylhexyl) sulfosuccinate      |
| Brij 35           | Polyoxyethylene(23) dodecyl ether    |
| BSA               | Bovine serum albumin                 |
| <i>tert</i> -BuOH | <i>tert</i> -Butyl alcohol           |
| CPC               | Hexadecylpyridinium chloride         |
| CTAB              | Hexadecyltrimethylammonium bromide   |
| CTAC              | Hexadecyltrimethylammonium chloride  |
| DAP               | Dodecylammonium propionate           |
| DDAB              | Didodecyldimethylammonium bromide    |
| diox              | Dioxane                              |
| dis               | dispersion                           |
| DMAA              | <i>N,N</i> -Dimethylacetamide        |
| DMF               | <i>N,N</i> -Dimethylformamide        |
| DODAC             | Dioctadecyldimethylammonium chloride |
| DPPC              | Dipalmitoyl phosphatidylcholine      |
| DTAC              | Dodecyltrimethylammonium chloride    |
| EtOH              | Ethanol                              |
| HSA               | Human serum albumin                  |
| MeOH              | Methanol                             |
| mic               | micelles                             |
| <i>i</i> -octane  | 2,2,4-Trimethylpentane               |
| 1-PrOH            | 1-Propanol                           |
| 2-PrOH            | 2-Propanol                           |
| PS                | Polystyrene                          |

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Table 1, Quantum yields of photosensitized production of singlet oxygen.

| No.                                  | Solvent                       | [O <sub>2</sub> ]     | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method               | Comment   | Ref.   |
|--------------------------------------|-------------------------------|-----------------------|-------------------|----------------|----------------|----------------------------|----------------------|---|--------|
| <b>1.1 2'-Acetonaphthone (2-ACN)</b> |                               |                       |                   |                |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | air or O <sub>2</sub> | 0.71              | 0.81           |                |                            |                      | See Table 4.  |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | air <sup>a</sup>      | 0.73 <sup>T</sup> | 0.87           |                |                            | CP/LI-56,42          | S' = 9-Fluorenone; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.84$ . $P_T^{O_2} = 1$ ; measured ratio of $I_a$ at $\lambda_{exc}(S) = 336$ and $\lambda_{exc}(S') = 367$ nm.   | 91F023 |
|                                      | C <sub>6</sub> H <sub>6</sub> | air                   | 0.59 <sup>T</sup> | 0.70           |                |                            | PL/LI,St-55,42       | S' = Ac; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.84^e$ . $\epsilon_T(S) = 10,500$ L mol <sup>-1</sup> cm <sup>-1</sup> at 430 nm, $\epsilon_T(S') = 24,300$ L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm, $P_T^{O_2}(S$ and S') = 1. | 84E373 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        | 0.73 <sup>T</sup> | 0.87           |                |                            | PL/Hp-52,42          | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.84$ . Measured $\phi_{\Delta} = 0.73$ , $P_T^{O_2} = 1$ and $\phi_F$ .  | 88E449 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        | 0.71 <sup>T</sup> | 0.85           |                |                            | PL/LI-56,42          | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.84$ . Measured $P_T^{O_2} = 1$ .  | 88E449 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        | 0.4 <sup>T</sup>  | 0.5            |                |                            | PR/Ad,St-49,42       | A = DPBF; used $\phi_T(S) = 0.84$ , $\epsilon_T(S) = 10,500$ L mol <sup>-1</sup> cm <sup>-1</sup> at 430 nm. Measured $G(^3S^*)$ .  | 78E263 |
|                                      | CD <sub>3</sub> OD            | air <sup>a</sup>      | 0.79 <sup>T</sup> |                |                |                            | CP/LI-56             | S' = RB; rel. to $\phi_{\Delta}(S') = 0.76$ . $P_T^{O_2} = 1$ ; meas. ratio of $I_a$ at $\lambda_{exc}(S) = 336$ and $\lambda_{exc}(S') = 547$ nm.  | 91F023 |
|                                      | MeOH                          | O <sub>2</sub>        | 0.75 <sup>T</sup> |                |                |                            | CP/Ac-15             | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ .  | 767071 |
| <b>1.2 Acetophenone (AP)</b>         |                               |                       |                   |                |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | air                   |                   | 0.35*          |                |                            | PL/LI,St-55,42       | S' = BP; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 1^e$ .   | 86A230 |
|                                      |                               |                       | 0.29 <sup>T</sup> | 0.29           |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | air <sup>a</sup>      | 0.41 <sup>T</sup> | 0.41           |                |                            | PL/ $\beta$ Cb-43,42 | S' = BP; TD = S; rel. to $f_{\Delta}^T(S') = 0.35$ ; used $\phi_T(S) = 1$ . Measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 1.2$ .   | 76F904 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        | 0.33 <sup>T</sup> | 0.33           |                |                            | PL/Hp-52,42          | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 1$ . Measured $\phi_{\Delta} = 0.31$ , $P_T^{O_2} = 0.94$ and $\phi_F$ .  | 88E449 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        | 0.36 <sup>T</sup> | 0.36           |                |                            | PL/LI-56,42          | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 1$ . Measured $P_T^{O_2} = 0.94$ .  | 88E449 |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        |                   | 0.31*          |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.39$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |
|                                      |                               |                       | 0.35 <sup>T</sup> | 0.35           |                |                            |                      |   |        |
|                                      | CH <sub>3</sub> CN            | O <sub>2</sub>        | 0.52 <sup>T</sup> | 0.52           |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.37$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |
|                                      | MeOH                          | O <sub>2</sub>        | <0.58             |                |                |                            | CP/Oc-14             | A = 2,5-DMF; $\lambda_{exc} = 283$ -373 nm. Some free radical reaction occurs.  | 70F735 |
| <b>1.3 Acetophenone, 4'-cyano-</b>   |                               |                       |                   |                |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        |                   | 0.44*          |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.39$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |
|                                      |                               |                       | 0.49 <sup>T</sup> | 0.49           |                |                            |                      |   |        |
|                                      | CH <sub>3</sub> CN            | O <sub>2</sub>        | 0.76 <sup>T</sup> | 0.76           |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.37$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |
| <b>1.4 Acetophenone, 3'-methoxy-</b> |                               |                       |                   |                |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | air                   |                   | 0.33*          |                |                            | PL/LI,St-55          | S' = BP; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm.  | 86A230 |
|                                      |                               |                       |                   | 0.27           |                |                            |                      |   |        |
| <b>1.5 Acetophenone, 4'-methoxy-</b> |                               |                       |                   |                |                |                            |                      |   |        |
|                                      | C <sub>6</sub> H <sub>6</sub> | O <sub>2</sub>        |                   | 0.24*          |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.39$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |
|                                      |                               |                       | 0.27 <sup>T</sup> | 0.27           |                |                            |                      |   |        |
|                                      | CH <sub>3</sub> CN            | O <sub>2</sub>        | 0.42 <sup>T</sup> | 0.42           |                |                            | PL/Ad,TAt-50,42      | S' = BP; A = DPBF; TA = 1-MeNp; rel. to $f_{\Delta}^T(S') = 0.37$ ; meas. $\phi_T(S) = 1^e$ ; $\lambda_{exc} = 337$ nm. Showed $P_T^{O_2}(S$ and S') > 0.95.  | 85A268 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                           | [O <sub>2</sub> ]          | $\phi_{\Delta}$   | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method         | Comment  | Ref.             |
|--|-----------------------------------|----------------------------|-------------------|-------------------|----------------|----------------------------|----------------|--|------------------|
| <b>1.6 Acetophenone, 2'-methyl-, biradical</b>               |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | CH <sub>3</sub> CN                | air <sup>a</sup>           |                   | 0.23 <sup>T</sup> | 0.38           |                            | PL/LI-56       | $S' = \text{Ac}$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{\text{exc}} = 337 \text{ nm}$ .<br>$f_{\Delta}^T$ based on quantum yield of biradical formation = 0.60 in soln. contg. 0.012 mol L <sup>-1</sup> 2-methylacetophenone.   | 89A241           |
| <b>1.7 Acridine (Ac)</b>                                     |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>     | air or O <sub>2</sub>      | 0.83              | 0.99              |                |                            |                | See Table 4.   |                  |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             | 0.84 <sup>T</sup> | 1                 |                |                            | PL/Hp-52,42    | $\lambda_{\text{exc}} = 355 \text{ nm}$ ; used $\phi_T(S) = 0.86^g$ . Measured $\phi_{\Delta} = 0.84$ , $P_T^{O_2} = 1$ and $\phi_F$ .   | 88E449           |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             | 0.84 <sup>T</sup> | 1                 |                |                            | PL/LI-56,42    | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.86^g$ . Measured $P_T^{O_2} = 1$ .  | 88E449           |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             | 0.6 <sup>T</sup>  | 0.7               |                |                            | PR/Ad,St-49,42 | A = DPBF; used $\phi_T(S) = 0.86^g$ , $\epsilon_T(S) = 24,300 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 440 nm. Measured $G(^3S^*)$ .   | 78E263           |
|  | CDCl <sub>3</sub>                 | $\sim 1.16 \times 10^{-2}$ | 0.95 <sup>T</sup> |                   |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{\text{exc}} = 337 \text{ nm}$ ; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 525 nm. $P_T^{O_2} = 1$ ; $p_A = 1$ .   | 87E410           |
|  | CH <sub>3</sub> CN                | O <sub>2</sub>             | 0.82 <sup>T</sup> |                   |                |                            | PL/Hp-52       | $\lambda_{\text{exc}} = 354 \text{ nm}$ .  | 88Z155           |
| <b>1.8 9-Acridinethione, 10-methyl- (NMTA)</b>               |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | c-C <sub>6</sub> H <sub>12</sub>  | O <sub>2</sub>             |                   | 1                 |                |                            | PL/Ad,St-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.79$ ; $\lambda_{\text{exc}} = 485 \text{ nm}$ ; used $k_d = 5.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 3.4 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(S) = 8800 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. Measured $P_T^{O_2}$ . | 84E342           |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             |                   | 0.92              |                |                            | PL/Ad,St-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.85$ ; $\lambda_{\text{exc}} = 485 \text{ nm}$ ; used $k_d = 4.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 8.0 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(S) = 9300 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. Measured $P_T^{O_2}$ . | 84E342           |
|  | CH <sub>3</sub> CN                | O <sub>2</sub>             |                   | 0.85              |                |                            | PL/Ad,St-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.76$ ; $\lambda_{\text{exc}} = 485 \text{ nm}$ ; used $k_d = 2.5 \times 10^4 \text{ s}^{-1}$ , $k_A = 1.0 \times 10^9 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(S) = 9000 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. Measured $P_T^{O_2}$ . | 84E342           |
|  | MeOH                              | O <sub>2</sub>             |                   | 1.0               |                |                            | PL/Ad,St-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.75$ ; $\lambda_{\text{exc}} = 485 \text{ nm}$ ; used $k_d = 1.0 \times 10^5 \text{ s}^{-1}$ , $k_A = 8.1 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(S) = 8500 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. Measured $P_T^{O_2}$ . | 84E342           |
| <b>1.9 Acridinium, 3,6-diamino- (Proflavine)</b>             |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | H <sub>2</sub> O                  | air <sup>a</sup>           | 0.12              | 0.25              |                |                            | CP/Ac-43,42    | $S' = \text{MB}^+$ ; A = 2,5-DMF; rel. to $\phi_{\Delta}(S') = 0.52$ ; used $\phi_T(S) = 0.47$ . Assumed $P_T^{O_2} = 1$ .   | 737339           |
| <b>1.10 Acridinium, 3,6-diamino-10-methyl- (Acriflavine)</b> |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | CH <sub>3</sub> COCH <sub>3</sub> | air <sup>a</sup>           |                   | 0.1               |                |                            | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ . Rel. to S' in CCl <sub>4</sub> .  | 82Z317           |
| <b>1.11 Allopsoralen (Furo[2,3-f]benzopyran-7-one)</b>       |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             | 0.08*             |                   |                |                            | PL/LI-56,42    | $S' = \text{Ac}$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.17$ ; $\lambda_{\text{exc}} = 355 \text{ nm}$ . $P_T^{O_2} = 1$ .   | 88E121           |
|  |                                   |                            | 0.07 <sup>T</sup> | 0.41              |                |                            |                |  |                  |
| <b>1.12 Angelicin (Furo[2,3-h]benzopyran-2-one, Ang)</b>     |                                   |                            |                   |                   |                |                            |                |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>             | 0.01 <sup>T</sup> | 0.33              |                |                            | PL/LI-56,42    | $S' = \text{Ac}$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.03$ ; $\lambda_{\text{exc}} = 355 \text{ nm}$ . $P_T^{O_2} = 1$ .   | 88E121           |
|  | CCl <sub>4</sub>                  | air                        | 0.002*            |                   |                |                            | MP/LI-56       | $S' = \text{TPP}$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{\text{exc}} = 652 \text{ nm}$ .  | 83E813           |
|  | D <sub>2</sub> O                  | air                        | 0.02 <sup>T</sup> |                   |                |                            | PL/LI-56       | $S' = \text{RF}$ ; rel. to $\phi_{\Delta}(S') = 0.3$ ; $\lambda_{\text{exc}} = 337 \text{ nm}$ .   | 86E959<br>86F144 |
|  | MeOH                              | air                        | 0.03 <sup>T</sup> | 1                 |                |                            | PL/LI-56,42    | $S' = \text{RF}$ ; rel. to $\phi_{\Delta}(S') = 0.4$ ; $\lambda_{\text{exc}} = 337 \text{ nm}$ ; used $\phi_T(S) = 0.31^d$ .   | 86E959<br>86F144 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.                         | Solvent   | [O <sub>2</sub> ]      | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|-----------------------------|---|------------------------|-------------------|----------------|----------------|----------------------------|-------------|--|--------|
| <b>1.13 Anthracene (An)</b> |   |                        |                   |                |                |                            |             |  |        |
|                             | iso-BuOH  | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.32$  | 87E668 |
|                             | 1-BuOH  | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.26$  | 87E668 |
|                             | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.35$  | 87E668 |
|                             | i-C <sub>5</sub> H <sub>11</sub> OH             | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.38$  | 87E668 |
|                             | n-C <sub>6</sub> H <sub>14</sub>                | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.68$  | 87E668 |
|                             | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | 0.2 atm O <sub>2</sub> | 0.83              |                |                |                            | PL/LI-38,56 | used $\phi_T(S) = 0.72$ . Assumed $f_T^{O_2} = 1$ ; used $f_{\Delta}^T = 1.0$ and $f_{\Delta}^S = 0.46$ .  | 87E668 |
|                             | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | O <sub>2</sub>         | 1.0               |                |                |                            | PL/LI-38,56 | used $\phi_T(S) = 0.72$ . Assumed $f_T^{O_2} = 1$ ; used $f_{\Delta}^T = 1.0$ and $f_{\Delta}^S = 0.46$ .  | 87E668 |
|                             | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | 1.2 × 10 <sup>-3</sup> |                   |                |                | 1.0                        | PL/Ad,St-48 | A = Rub; $\lambda_{exc} = 347 \text{ nm}$ ; used $\phi_A(S) = 0.72$ , $\epsilon_T(S) = 42,000 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 428.5 nm. $P_T^{O_2} = 1$ ; $n_{\Delta} = 1$ .  | 83F075 |
|                             | C <sub>6</sub> H <sub>5</sub> CN                | 1.2 × 10 <sup>-3</sup> |                   |                |                | 0.57                       | PL/Ad,St-48 | A = Rub; $\lambda_{exc} = 347 \text{ nm}$ ; used $\phi_T(S) = 0.72$ . $P_T^{O_2} = 1$ ; used $\epsilon_T(S) = 24,000 \text{ L mol}^{-1} \text{ cm}^{-1}$ at $\lambda_{max}$ ; $n_{\Delta} = 0.57$ .  | 83F075 |
|                             | C <sub>6</sub> H <sub>5</sub> Cl                | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.95$  | 87E668 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.85$  | 87E668 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | 1.3 × 10 <sup>-4</sup> | 0.58 <sup>T</sup> | 0.77           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; $\lambda_{exc} = 355 \text{ nm}$ ; used $\phi_T(S) = 0.75$ . $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .   | 88E452 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | air                    | ~0.74             |                |                |                            | PL/Hp-52,42 | $\lambda_{exc} = 337 \text{ nm}$ . Measured $\phi_T$ ; assumed $P_T^{O_2} = 1$ , [S] > 5 × 10 <sup>-4</sup> mol L <sup>-1</sup> , used $\phi_F = 0.22$ ; $\phi_{\Delta} = 0.50$ extrapolating [S] → 0; authors used meas. $\phi_T$ to give $f_{\Delta}^T = 0.95$ but $P_S^{O_2} \neq 0$ .                          | 91F198 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | air                    | 0.61              |                |                |                            | PL/Hp-52    | $\lambda_{exc} = 355 \text{ nm}$ . Assumed $f_{\Delta}^S = 0$ ; $\phi_T^{O_2} = 0.78$ gives $f_{\Delta}^T = 0.78$ .  | 85E591 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | air <sup>a</sup>       | 0.63              |                |                |                            | PL/βCb-43   | S' = BP; rel. to $\phi_{\Delta}(S') = 0.35$ . Measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 1.8$ ; since $P_S^{O_2} \neq 0$ , only $\phi_{\Delta}$ is obtainable.   | 76F904 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | 1.9 × 10 <sup>-3</sup> | 0.88              |                |                |                            | CP/Ac-46    | S' = A = DMA; rel. to $\phi_{\Delta}(S') = 0.52$ ; $\lambda_{exc} = 365 \text{ nm}$ . Assumed $f_T^{O_2} = 1$ .  | 81F364 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | O <sub>2</sub>         | 0.68              |                |                |                            | PL/Hp-52    | $\lambda_{exc} = 355 \text{ nm}$ ; used $\phi_T(S) = 0.78$ . Measured $\phi_{\Delta} = 0.68$ , $P_T^{O_2} = 1$ and $\phi_T^{O_2} = \phi_T(S)$ and $\phi_F$ . Authors assume $f_{\Delta}^S = 0$ and $f_{\Delta}^T = 0.87$ but $P_S^{O_2} = 0.52$ so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable. | 88E449 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | O <sub>2</sub>         | 0.63              |                |                |                            | PL/LI-56    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ . Measured $P_T^{O_2} = 1$ and $\phi_T^{O_2} \approx \phi_T(S)$ . Authors assume $f_{\Delta}^S = 0$ and $f_{\Delta}^T = 0.87$ but $P_S^{O_2} = 0.52$ so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable.  | 88E449 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | O <sub>2</sub>         |                   | 0.7            |                |                            | PR/Ad,St-49 | A = DPBF; used $\phi_T(S) = 0.75$ , $\epsilon_T(S) = 45,500 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 432 nm. Measured $G(^3S^*)$ .   | 78E263 |
|                             | C <sub>6</sub> H <sub>6</sub>                   | 9.0 × 10 <sup>-3</sup> | 1.1               | 1.0            | 0.46           |                            | CP/Ac-46,38 | S' = A = DMA; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 365 \text{ nm}$ ; used $\phi_T(S) = 0.74$ . Assumed $f_T^{O_2} = 1$ ; $\phi_{\Delta}(S') = 1$ through coronene using $\phi_{\Delta}(\text{ave.}) = 0.88$ .  | 81F364 |
|                             | n-C <sub>7</sub> H <sub>16</sub>                | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.63$  | 87E668 |
|                             | CCl <sub>4</sub>                                | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.075$   | 87E668 |
|                             | CCl <sub>4</sub>                                | air                    | 0.13*             |                |                |                            | MP/LI-56    | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.7$ .  | 86E959 |
|                             | CCl <sub>4</sub>                                | O <sub>2</sub>         | 0.75              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365 \text{ nm}$ .  | 537004 |
|                             | CH <sub>2</sub> Cl <sub>2</sub>                 | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.37$  | 87E668 |
|                             | CH <sub>3</sub> CN                              | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.27$  | 87E668 |
|                             | CH <sub>3</sub> COCH <sub>3</sub>               | 0.2 atm O <sub>2</sub> |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.45$  | 87E668 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]       | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|---|---|-------------------------|-------------------|----------------|----------------|----------------------------|-------------|--|--------|
| <b>1.13 Anthracene (An)—Continued</b>       |   |                         |                   |                |                |                            |             |  |        |
|   | CHCl <sub>3</sub>                                       | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.62$  | 87E668 |
|   | CHCl <sub>3</sub>                                       | O <sub>2</sub>          | 0.69              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CS <sub>2</sub>   | O <sub>2</sub>          | 0.70              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | DMF   | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.36$  | 87E668 |
|   | EtOH  | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.26$  | 87E668 |
|   | HCONH <sub>2</sub>                                      | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.20$  | 87E668 |
|   | MeOH  | air                     | 0.7               |                |                |                            | PL/LI-56    | S' = RF; rel. to $\phi_{\Delta}(S') = 0.4$ .   | 86E959 |
|   | 1-PrOH  | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.3$   | 87E668 |
|   | 2-PrOH  | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.32$  | 87E668 |
|   | c-C <sub>4</sub> H <sub>8</sub> O                       | 0.2 atm O <sub>2</sub>  |                   |                |                |                            | PL/LI-56    | $\phi_{\Delta}(\tau_r(\text{toluene})/\tau_r) = 0.44$  | 87E668 |
| <b>1.14 Anthracene, 1-chloro-</b>           |   |                         |                   |                |                |                            |             |  |        |
|   | CCl <sub>4</sub>  | O <sub>2</sub>          | 0.45              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CHCl <sub>3</sub>                                       | O <sub>2</sub>          | 0.66              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CS <sub>2</sub>   | O <sub>2</sub>          | 0.64              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
| <b>1.15 Anthracene, 9-chloro-</b>           |   |                         |                   |                |                |                            |             |  |        |
|   | CCl <sub>4</sub>  | O <sub>2</sub>          | 0.63              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CHCl <sub>3</sub>                                       | O <sub>2</sub>          | 0.56              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CS <sub>2</sub>   | O <sub>2</sub>          | 0.57              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
| <b>1.16 Anthracene, 9-cyano-</b>            |   |                         |                   |                |                |                            |             |  |        |
|   | C <sub>6</sub> H <sub>6</sub> and<br>CH <sub>3</sub> CN | air and O <sub>2</sub>  | ~2 <sup>ST</sup>  | ~1             | ~1             |                            | CP/Pa-14    | $\lambda_{\text{exc}} = 365$ nm. A = TME, 2M2B, or cyclohexene, P = alkene hydroperoxides, solvent = C <sub>6</sub> H <sub>6</sub> and CH <sub>3</sub> CN.   | 85F160 |
| <b>1.17 Anthracene, 9,10-dibromo-</b>       |   |                         |                   |                |                |                            |             |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                           | air                     | -0.85             | -0.96          |                |                            | PL/Hp-52,42 | $\lambda_{\text{exc}} = 337, 400$ nm. Measured $\phi_T$ ; [S] > 5 × 10 <sup>-4</sup> mol L <sup>-1</sup> , assumed $P_T^{O_2} = 1$ , used $\phi_F = 0.11$ ; $\phi_{\Delta} = 0.44$ , $f_{\Delta}^T = 0.49$ extrapolating [S] → 0.            | 91F198 |
| <b>1.18 Anthracene, 9,10-dichloro-</b>      |   |                         |                   |                |                |                            |             |  |        |
|   | CCl <sub>4</sub>  | O <sub>2</sub>          | 0.89              |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CHCl <sub>3</sub>                                       | O <sub>2</sub>          | 1.6               |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
|   | CS <sub>2</sub>   | O <sub>2</sub>          | 2.0               |                |                |                            | CP/Oc-14    | A = S; $\lambda_{\text{exc}} = 365$ nm.  | 537004 |
| <b>1.19 Anthracene, 9,10-dicyano- (DCA)</b> |   |                         |                   |                |                |                            |             |  |        |
|   | c-C <sub>6</sub> H <sub>12</sub>                        | → ∞                     | 1.9 <sup>ST</sup> |                |                |                            | PL/LI-56    | S' = Py; rel. to $\phi_{\Delta}(S') = 0.81$ ; $\lambda_{\text{exc}} = 355$ nm.   | 91E297 |
|   | C <sub>6</sub> H <sub>6</sub>                           | air                     | 0.19              |                |                |                            | CP/LI-56    | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.67$ .   | 89E223 |
|   |   |                         |                   |                |                |                            |             |  | 88E609 |
|   | C <sub>6</sub> H <sub>6</sub>                           | air                     | 0.48              |                |                |                            | CP/Ac-14    | A = MDH. $f_r^A = 0.30$ .  | 89E223 |
|   | C <sub>6</sub> H <sub>6</sub>                           | 1.45 × 10 <sup>-3</sup> | 0.28              |                |                |                            | CP/Ac-14,38 | A = 2M2P. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ .  | 83F172 |
|   | C <sub>6</sub> H <sub>6</sub>                           | 6.8 × 10 <sup>-3</sup>  | 0.82              |                |                | 1.7                        | CP/Ac-14,38 | A = 2M2P; $\lambda_{\text{exc}} = 334, 366$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ .  | 83F172 |
|   | C <sub>6</sub> H <sub>6</sub>                           | → ∞                     | 1.6 <sup>ST</sup> | 0.70           | 0.86           |                            | PL/LI-56,38 | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{\text{exc}} = 355$ nm. Used $P_T^{O_2} = 1$ ; $f_{\Delta}^T$ was measured using 2,5-dimethyliodobenzene enhanced intersystem crossing producing <sup>3</sup> S* with 50% efficiency. | 92F013 |
|   | C <sub>6</sub> D <sub>6</sub>                           | 1.45 × 10 <sup>-3</sup> | 0.46              |                |                |                            | PL/LI-38,56 | S' = DNT; rel. to $\phi_{\Delta}(S') = 0.98$ ; $\lambda_{\text{exc}} = 355$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ , $f_T^{O_2} = 1$ .  | 83F172 |
|   | C <sub>6</sub> D <sub>6</sub>                           | 6.8 × 10 <sup>-3</sup>  | 1.1               |                |                | 1.6                        | PL/LI-38,56 | S' = DNT; rel. to $\phi_{\Delta}(S') = 0.98$ ; $\lambda_{\text{exc}} = 355$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ , $f_T^{O_2} = 1$ .  | 83F172 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]        | $\phi_{\Delta}$   | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method  | Comment  | Ref.             |
|---|---|--------------------------|-------------------|-------------------|----------------|----------------------------|---|--|------------------|
| <b>1.19 Anthracene, 9,10-dicyano- (DCA)—Continued</b>     |   |                          |                   |                   |                |                            |   |  |                  |
|   | C <sub>6</sub> H <sub>6</sub> and CH <sub>3</sub> CN          | air and O <sub>2</sub>   | -2 <sup>ST</sup>  | -1                | -1             |                            | CP/Pa-14  | $\lambda_{exc} = 365$ nm. A = TME, 2M2B, or cyclohexene, P = alkene hydroperoxides, solvent = C <sub>6</sub> H <sub>6</sub> and CH <sub>3</sub> CN.                                    | 85F160           |
|   | CCl <sub>4</sub>  | air                      | 0.15*             | 0.13              |                |                            | CP/LI-56  | S' = TPP; A = MDH; rel. to $\phi_{\Delta}(S') = 0.54$ .  | 89E223           |
|   | CCl <sub>4</sub>  | air                      | 0.16              |                   |                |                            | CP/Ac-14  | A = MDH. $f_r^A = 0.30$ .  | 89E223           |
|   | CCl <sub>4</sub>  | O <sub>2</sub>           | 2 <sup>ST</sup>   |                   |                |                            | CP/Pa-14  | A = DPB. $P_T^{O_2} = 1$ .   | 90F292           |
|   | CH <sub>3</sub> CN  | air                      | 0.23              |                   |                |                            | CP/LI-56  | S' = TPP; A = MDH; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 89E223           |
|   | CH <sub>3</sub> CN  | air                      | 0.76              |                   |                |                            | CP/Ac-14  | A = MDH. $f_r^A = 0.30$ .  | 89E223           |
|   | CH <sub>3</sub> CN  | 1.7 × 10 <sup>-3</sup>   | 0.06              |                   |                |                            | CP/Ac-14,38   | Δ = 2M2P; $\lambda_{exc} = 334, 366$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ .   | 83F172           |
|   | CH <sub>3</sub> CN  | 8.1 × 10 <sup>-3</sup>   | 0.25              |                   | 2.0            |                            | CP/Ac-14,38   | A = 2M2P; $\lambda_{exc} = 334, 366$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0$ .   | 83F172           |
|   | CH <sub>3</sub> CN  | → ∞                      | 1.5 <sup>ST</sup> |                   | 0.76           |                            | PL/LI-56  | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm. Assumed $f_{\Delta}^T = 0.7, f_T^{O_2} = 1$ .  | 92F013           |
|   | CD <sub>3</sub> CN  | 1.7 × 10 <sup>-3</sup>   | 0.90              |                   |                |                            | PL/LI-38,56   | S' = DNT; rel. to $\phi_{\Delta}(S') = 0.62$ ; $\lambda_{exc} = 355$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0, f_T^{O_2} = 1$ .  | 83F172           |
|   | CD <sub>3</sub> CN  | 8.1 × 10 <sup>-3</sup>   | 1.6               |                   | 2.0            |                            | PL/LI-38,56   | S' = DNT; rel. to $\phi_{\Delta}(S') = 0.62$ ; $\lambda_{exc} = 355$ nm. Used $P_T^{O_2} = 1$ , assumed $\phi_T = 0, f_T^{O_2} = 1$ .  | 83F172           |
|   | CHCl <sub>3</sub>   | air                      | 0.16              |                   |                |                            | CP/Ac-14  | A = MDH. $f_r^A = 0.30$ .  | 89E223           |
|   | CHCl <sub>3</sub>   | air                      | 0.09              |                   |                |                            | CP/LI-56  | S' = TPP; A = MDH; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 89E223           |
|   | CS <sub>2</sub>   | air                      | 0.09              |                   |                |                            | CP/LI-56  | S' = TPP; A = MDH; rel. to $\phi_{\Delta}(S') = 0.51$ .  | 89E223           |
|   | CS <sub>2</sub>   | air                      | 0.17              |                   |                |                            | CP/Ac-14  | A = MDH. $f_r^A = 0.30$ .  | 89E223           |
|   | ClCF <sub>2</sub> CCl <sub>2</sub> F                          | air                      | 0.14              |                   |                |                            | CP/Ac-14  | A = MDH. $f_r^A = 0.30$ .  | 89E223           |
|   | ClCF <sub>2</sub> CCl <sub>2</sub> F                          | air                      | 0.09              |                   |                |                            | CP/LI-56  | S' = TPP; A = MDH; rel. to $\phi_{\Delta}(S') = 0.41$ .  | 89E223           |
| <b>1.20 Anthracene, 1,4-dimethoxy-9,10-diphenyl-</b>      |   |                          |                   |                   |                |                            |   |  |                  |
|   | (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> O               | (2-9) × 10 <sup>-3</sup> |                   |                   | 0.69           | CP/Ac-14,38                | A = S. Assumed $f_T^{O_2} = 1, \phi_f_{\Delta}^T \approx 0$ . | 84F197   |                  |
|   | CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> | (2-9) × 10 <sup>-3</sup> |                   |                   | 0.69           | CP/Ac-14,38                | A = S. Assumed $f_T^{O_2} = 1, \phi_f_{\Delta}^T = 0.08$ .    | 84F197   |                  |
| <b>1.21 Anthracene, 9,10-dimethyl- (DMA)</b>              |   |                          |                   |                   |                |                            |   |  |                  |
|   | C <sub>5</sub> H <sub>5</sub> N                               | O <sub>2</sub>           | 0.19              |                   |                |                            | CP/Oc-14  | A = H <sub>2</sub> NCSNH <sub>2</sub> ; $\lambda_{exc} = 405$ nm. Assumed $f_r^A = 2$ .  | 737347<br>74E522 |
|   | n-C <sub>6</sub> H <sub>14</sub>                              | O <sub>2</sub>           | 1.1               | ≥0.42             | ≥0.41          |                            | CP/Ac-27  | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ ; used $p_A = 1$ .  | 79E643           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                 | (2-9) × 10 <sup>-3</sup> |                   |                   | 2.0            | CP/Ac-14,38                | A = S. Assumed $f_T^{O_2} = 1, \phi_f_{\Delta}^T = 0.05$ .    | 84F197   |                  |
|   | C <sub>6</sub> H <sub>6</sub>                                 | air <sup>a</sup>         | 0.08 <sup>T</sup> | 1                 | 1              | 2.0                        | CP/Ac-14,40   | A = S. Assumed $f_T^{O_2} = 1; f_{\Delta}^T + f_{\Delta}^S$ from $\phi_{\Delta}$ when $P_S^{O_2} = 1$ ; $\phi_f_{\Delta}^T = \phi_{\Delta}$ when $P_S^{O_2} = 0$ .                     | 76F422           |
|   | C <sub>6</sub> H <sub>6</sub>                                 | air <sup>a</sup>         |                   |                   | ≥0.62          | ≥1.6                       | CP/Ac-14,38   | A = S. Assumed $f_{\Delta}^T = 1$ and $f_T^{O_2} = 1$ .  | 76F905           |
|   | C <sub>6</sub> H <sub>6</sub>                                 | O <sub>2</sub> var.      |                   |                   |                |                            | CP/Ac-14,38   | A = S; $\lambda_{exc} = 365$ nm. $\phi_f_{\Delta}^T / (f_{\Delta}^T + f_{\Delta}^S) = 0.02 \pm 0.05$ .   | 68F286           |
|   | C <sub>6</sub> H <sub>6</sub>                                 | 1.9 × 10 <sup>-3</sup>   | 0.52              |                   |                |                            | CP/Ac-14  | A = S; $\lambda_{exc} = 365$ nm. Assumed $f_T^{O_2} = 1$ ; measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.56, 0.59$ and 0.91 for S' = Cor, An and BP, resp.                          | 81F364           |
|   | C <sub>6</sub> H <sub>6</sub>                                 | 9.0 × 10 <sup>-3</sup>   | 1.0               |                   |                | 1.4                        | CP/Ac-14  | A = S; $\lambda_{exc} = 365$ nm; used $\phi_T(S) = -0.02$ . Assumed $f_T^{O_2} = 1$ ; measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 1.1, 0.91$ and 1.1 for S' = Cor, An and BP, resp. | 81F364           |
| <b>1.22 Anthracene, 2-(3,3-dimethyl-1-butenyl)-, (E)-</b> |   |                          |                   |                   |                |                            |   |  |                  |
|   | C <sub>6</sub> H <sub>6</sub>                                 | 1.3 × 10 <sup>-4</sup>   | 0.46*             | 0.38 <sup>T</sup> | 0.76           |                            | PL/LI-56,42   | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.46$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .   | 88E452           |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]             | $\phi_{\Delta}$            | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.   |
|------|--|-------------------------------|----------------------------|----------------|----------------|----------------------------|-------------|---|--------|
| 1.23 | Anthracene, 2-(3,3-dimethyl-1-butenyl)-, (Z)-<br>C <sub>6</sub> H <sub>6</sub> | $1.3 \times 10^{-4}$          | 0.63*<br>0.52 <sup>T</sup> | 0.88           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.59$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .  | 88E452 |
| 1.24 | Anthracene, 9-(1,1-dimethylethyl)-<br>H <sub>2</sub> O (mic)<br>pH = 7         | air <sup>a</sup>              |                            |                |                |                            | CP/Pa-43    | S' = An; A = Im; P = Imidazole endoperoxide; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.06$ . soln. cont. 1% CTAB, RNO as monitor of P.  | 83N082 |
| 1.25 | Anthracene, 9,10-diphenyl-<br>n-C <sub>6</sub> H <sub>14</sub>                 | O <sub>2</sub>                | 1.1                        | $\geq 0.49$    | $\geq 0.48$    |                            | CP/Ac-27    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ ; used $p_A = 1$ .   | 79E643 |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                  | $(2\text{-}9) \times 10^{-3}$ |                            |                | 0.8            |                            | CP/Ac-14,38 | A = S. Assumed $f_T^{O_2} = 1$ , $\phi_T f_{\Delta}^T = 0.08$ .   | 84F197 |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                  | $(2\text{-}9) \times 10^{-3}$ | 2 <sup>ST</sup>            | 1              | 1              | 2                          | PL/Ad/St-48 | A = Rub; AC = S; $\lambda_{exc} = 347$ nm; used $k_d = 3.2 \times 10^4$ s <sup>-1</sup> , $k_A = 2.5 \times 10^7$ L mol <sup>-1</sup> s <sup>-1</sup> , $\epsilon_T(AC) = 12,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 450 nm. $P_T^{O_2} = 1$ ; measured $n_A = 2$ , thus $f_T^{O_2} = 1$ . | 82E451 |
|      | C <sub>6</sub> H <sub>6</sub>  | air                           | 0.13 <sup>T</sup>          | 1              |                |                            | CP/Ac-14,40 | A = S; $\lambda_{exc} = 436$ nm. $P_S^{O_2} = 0$ ; measured $\phi_T f_{\Delta}^T = 0.13$ .  | 727196 |
|      | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>              | 1 <sup>ST</sup>            |                |                |                            | CP/Pa-14,38 | A = S; $\lambda_{exc} = 436$ nm. $P_S^{O_2} = 1$ , measured $f_{\Delta}^T + f_{\Delta} S f_T^{O_2} = 1$ .   | 727196 |
|      | CCl <sub>4</sub>   | O <sub>2</sub>                | 0.75                       |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
|      | CHCl <sub>3</sub>  | O <sub>2</sub>                | 0.69                       |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
|      | CS <sub>2</sub>  | O <sub>2</sub>                | 1.8                        |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
| 1.26 | Anthracene, 9-methyl-<br>n-C <sub>6</sub> H <sub>14</sub>                      | O <sub>2</sub>                | 0.97                       | $\geq 0.32$    | $\geq 0.19$    |                            | CP/Ac-27    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ ; used $p_A = 1$ .   | 79E643 |
|      | CCl <sub>4</sub>   | O <sub>2</sub>                | 1.3                        |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
|      | CHCl <sub>3</sub>  | O <sub>2</sub>                | 1.2                        |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
| 1.27 | Anthracene, 2-[2-(2-naphthyl)ethenyl]-, (E)-<br>C <sub>6</sub> H <sub>6</sub>  | $1.3 \times 10^{-4}$          | 0.13*<br>0.11 <sup>T</sup> | 0.92           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.12$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .  | 88E452 |
| 1.28 | Anthracene, 2-[2-(2-naphthyl)ethenyl]-, (Z)-<br>C <sub>6</sub> H <sub>6</sub>  | $1.3 \times 10^{-4}$          | 0.12*<br>0.10 <sup>T</sup> | 0.45           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.22$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .  | 88E452 |
| 1.29 | Anthracene, 9-phenyl-<br>n-C <sub>6</sub> H <sub>14</sub>                      | O <sub>2</sub>                | 1.1                        | $\geq 0.50$    | $\geq 0.42$    |                            | CP/Ac-27    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ ; used $p_A = 1$ .   | 79E643 |
|      | CCl <sub>4</sub>   | O <sub>2</sub>                | 0.85                       |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
|      | CHCl <sub>3</sub>  | O <sub>2</sub>                | 0.94                       |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
|      | CS <sub>2</sub>  | O <sub>2</sub>                | 0.91                       |                |                |                            | CP/Oc-14    | A = S; $\lambda_{exc} = 365$ nm.  | 537004 |
| 1.30 | Anthracene, 2-(2-phenylethenyl)-, (Z)-<br>C <sub>6</sub> H <sub>6</sub>        | $1.3 \times 10^{-4}$          | 0.10*<br>0.08 <sup>T</sup> | 0.47           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.17$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .  | 88E452 |
| 1.31 | Anthracene, 2-(2-phenylethenyl)-, (E)-<br>C <sub>6</sub> H <sub>6</sub>        | $1.3 \times 10^{-4}$          | 0.12*<br>0.10 <sup>T</sup> | 0.91           |                |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.11$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .  | 88E452 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent   | [O <sub>2</sub> ]        | $\phi_{\Delta}$    | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.   |
|------|---|--------------------------|--------------------|-------------------|----------------|----------------------------|-------------|---|--------|
| 1.32 | Anthracene, 2-(1-propenyl)-, (E)-                             |                          |                    |                   |                |                            |             |   |        |
|      | C <sub>6</sub> H <sub>6</sub>                                 | 1.3 × 10 <sup>-4</sup>   | 0.50*              | 0.41 <sup>T</sup> | 0.89           |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.46$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .      | 88E452 |
| 1.33 | Anthracene, 2,6,9,10-tetracyano-                              |                          |                    |                   |                |                            |             |   |        |
|      | C <sub>6</sub> H <sub>6</sub> and CH <sub>3</sub> CN          | air and O <sub>2</sub>   | ~2 <sup>ST</sup>   | ~1                | ~1             |                            | CP/Pa-14    | $\lambda_{exc} = 365$ nm. A = TME, 2M2B, or cyclohexene, P = alkene hydroperoxides, solvent = C <sub>6</sub> H <sub>6</sub> and CH <sub>3</sub> CN. | 85F160 |
| 1.34 | Anthracene, 2-vinyl-  |                          |                    |                   |                |                            |             |   |        |
|      | C <sub>6</sub> H <sub>6</sub>                                 | 1.3 × 10 <sup>-4</sup>   | 0.43*              | 0.36 <sup>T</sup> | 0.73           |                            | PL/LI-56,42 | S' = BP; rel. to $\phi_{\Delta}(S') = 0.29$ ; meas. $\phi_T(S) = 0.49$ ; $\lambda_{exc} = 355$ nm. $P_S^{O_2} < 0.02$ and $P_T^{O_2} > 0.99$ .      | 88E452 |
| 1.35 | 1-Anthracesulfonate ion                                       |                          |                    |                   |                |                            |             |   |        |
|      | H <sub>2</sub> O  | 3 × 10 <sup>-3</sup>     | 0.70               | ~1                |                |                            | CP/Ac-14    | A = S. Assumed $P_T^{O_2} = 1$ and $f_{\Delta}^S = 0$ ; $\phi_T(\text{calc.}) = 0.82$ , $T = 30^\circ\text{C}$ .                                    | 78A275 |
| 1.36 | 2-Anthracesulfonate ion                                       |                          |                    |                   |                |                            |             |   |        |
|      | H <sub>2</sub> O  | 3 × 10 <sup>-3</sup>     | 0.70               | ~1                |                |                            | CP/Ac-14    | A = S. Assumed $P_T^{O_2} = 1$ and $f_{\Delta}^S = 0$ ; $\phi_T(\text{calc.}) = 0.81$ , $T = 30^\circ\text{C}$ .                                    | 78A275 |
| 1.37 | Anthra[1,9-bc:4,10-b'c']dichromene (ADC)                      |                          |                    |                   |                |                            |             |   |        |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                 | (2-9) × 10 <sup>-3</sup> |                    |                   | 0.8            |                            | CP/Ac-14,38 | A = S. Assumed $f_T^{O_2} = 1$ , $\phi_T f_{\Delta}^T = 0.01$ .   | 84F197 |
| 1.38 | Anthra[2,1,0-def:6,5,10-d'e'f']diisoquinoline, N,N'-dimethyl- |                          |                    |                   |                |                            |             |   |        |
|      | D <sub>2</sub> O  | O <sub>2</sub>           | 0.08               |                   |                |                            | PL/LI-56    | S' = ZnTMPyP <sup>4+</sup> ; rel. to $\phi_{\Delta}(S') = 0.88$ ; meas. $\phi_T(S) = 0.12$ ; $\lambda_{exc} = 355$ nm.                              | 91R201 |
| 1.39 | 9,10-Anthaquinone   |                          |                    |                   |                |                            |             |   |        |
|      | C <sub>6</sub> H <sub>6</sub>                                 | O <sub>2</sub>           | 0.15 <sup>T</sup>  | 0.17              |                |                            | PL/LI-56,42 | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.90$ . Measured $P_T^{O_2} = 0.65$ .   | 88E449 |
|      | C <sub>6</sub> H <sub>6</sub>                                 | O <sub>2</sub>           | 0.26 <sup>T</sup>  | 0.29              |                |                            | PL/Hp-52,42 | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.90$ . Measured $\phi_{\Delta} = 0.17$ , $P_T^{O_2} = 0.65$ and $\phi_T$ .                             | 88E449 |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.01 <sup>T</sup>  |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |
| 1.40 | 9,10-Anthaquinone, 1-amino-                                   |                          |                    |                   |                |                            |             |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.2 <sup>T</sup>   |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |
|      | 2-PrOH/<br>H <sub>2</sub> O (5:1)                             | air                      | 0.19 <sup>T</sup>  |                   |                |                            | CP/Ac-43    | S' = 1,5-AQ(NH <sub>2</sub> ) <sub>2</sub> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{exc} = 434$ nm.                               | 88F582 |
| 1.41 | 9,10-Anthaquinone, 2-amino-                                   |                          |                    |                   |                |                            |             |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.02 <sup>T</sup>  |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |
|      | 2-PrOH/<br>H <sub>2</sub> O (5:1)                             | air                      | 0.02 <sup>T</sup>  |                   |                |                            | CP/Ac-43    | S' = 1,5-AQ(NH <sub>2</sub> ) <sub>2</sub> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{exc} = 434$ nm.                               | 88F582 |
| 1.42 | 9,10-Anthaquinone, 1-amino-2-hydroxy-                         |                          |                    |                   |                |                            |             |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.02 <sup>T</sup>  |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |
| 1.43 | 9,10-Anthaquinone, 1-amino-4-hydroxy-                         |                          |                    |                   |                |                            |             |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.02 <sup>T</sup>  |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |
|      | MeOH  | O <sub>2</sub>           | 0.004 <sup>T</sup> |                   |                |                            | CP/Ac-43    | S' = RB; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{exc} = 546$ nm. Measured $P_T^{O_2} = 1$ .                           | 80F304 |
|      | 2-PrOH/<br>H <sub>2</sub> O (5:1)                             | air                      | 0.02 <sup>T</sup>  |                   |                |                            | CP/Ac-43    | S' = 1,5-AQ(NH <sub>2</sub> ) <sub>2</sub> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{exc} = 545$ nm.                               | 88F582 |
| 1.44 | 9,10-Anthaquinone, 1-amino-4-hydroxy-2-phenoxy-               |                          |                    |                   |                |                            |             |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>         | 0.05 <sup>T</sup>  |                   |                |                            | PL/LI-56    | S' = MPDME; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .  | 86E640 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                       | [O <sub>2</sub> ] | $\phi_{\Delta}$ | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method   | Comment  | Ref.   |
|--|-------------------------------|-------------------|-----------------|-------------------|----------------|----------------------------|----------|--|--------|
| <b>1.44 9,10-Anthraquinone, 1-amino-4-hydroxy-2-phenoxy</b> —Continued                 |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.05 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDEE}$ ; rel. to $\phi_{\Delta}(S') = 0.77$ . $P_T^{O_2} = 1$ .   | 82F631 |
|  | EtOH                          | air <sup>a</sup>  |                 | 0.05 <sup>T</sup> |                |                            | CP/Oc-43 | $S' = \text{MPDEE}$ ; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to $\phi_{\Delta}(S') = 0.77$ . Assumed $P_T^{O_2} = 1$ , $P_S^{O_2} = 0$ . | 82F631 |
| <b>1.45 9,10-Anthraquinone, 1-amino-4-hydroxy-2-[4-(phenylaminosulfonyl)phenoxy]</b> — |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.04 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.04 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDEE}$ ; rel. to $\phi_{\Delta}(S') = 0.77$ . $P_T^{O_2} = 1$ .   | 82F631 |
|  | EtOH                          | air <sup>a</sup>  |                 | 0.05 <sup>T</sup> |                |                            | CP/Oc-43 | $S' = \text{MPDEE}$ ; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to $\phi_{\Delta}(S') = 0.77$ . Assumed $P_T^{O_2} = 1$ , $P_S^{O_2} = 0$ . | 82F631 |
| <b>1.46 9,10-Anthraquinone, 1-amino-2-methyl-</b>                                      |                               |                   |                 |                   |                |                            |          |  |        |
|  | CCl <sub>4</sub>              | air               |                 | 0.12 <sup>T</sup> |                |                            | MP/LI-56 | $S' = \text{TPBC}$ ; rel. to $\phi_{\Delta}(S') = 0.45$ .  | 82A384 |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.12 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.47 9,10-Anthraquinone, 1-chloro-</b>  |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0                 |                |                            | PL/LI-56 | $S' = \text{MPDME}$ . $P_T^{O_2} = 1$ .  | 86E640 |
| <b>1.48 9,10-Anthraquinone, 2-chloro-</b>  |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0                 |                |                            | PL/LI-56 | $S' = \text{MPDME}$ . $P_T^{O_2} = 1$ .  | 86E640 |
| <b>1.49 9,10-Anthraquinone, 1,2-diamino-</b>   |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.03 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air               |                 | <0.05             |                |                            | CP/Pa-14 | A = DMA; P = 9,10-Dimethylanthracene endoperoxide; $\lambda_{\text{exc}} = 435$ nm. $P_T^{O_2} = 1$ .  | 80E446 |
|  | 2-PrOH/H <sub>2</sub> O (5:1) | air               |                 | 0.04 <sup>T</sup> |                |                            | CP/Ac-43 | $S' = 1,5\text{-AQ(NH}_2\text{)}_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 545$ nm.                          | 88F582 |
| <b>1.50 9,10-Anthraquinone, 1,4-diamino-</b>   |                               |                   |                 |                   |                |                            |          |  |        |
|  | CCl <sub>4</sub>              | air               |                 | 0.04 <sup>T</sup> |                |                            | MP/LI-56 | $S' = \text{TPBC}$ ; rel. to $\phi_{\Delta}(S') = 0.45$ .  | 82A384 |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.01 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air               |                 | <0.05             |                |                            | CP/Pa-14 | A = DMA; P = 9,10-Dimethylanthracene endoperoxide; $\lambda_{\text{exc}} = 435$ nm. $P_T^{O_2} = 1$ .  | 80E446 |
|  | 2-PrOH/H <sub>2</sub> O (5:1) | air               |                 | 0.03 <sup>T</sup> |                |                            | CP/Ac-43 | $S' = 1,5\text{-AQ(NH}_2\text{)}_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 545$ nm.                          | 88F582 |
| <b>1.51 9,10-Anthraquinone, 1,5-diamino-</b>   |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.46 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air               |                 | 0.67 <sup>T</sup> |                |                            | CP/Pa-14 | A = DMA; P = 9,10-Dimethylanthracene endoperoxide; $\lambda_{\text{exc}} = 435$ nm. $P_T^{O_2} = 1$ .  | 80E446 |
|  | 2-PrOH/H <sub>2</sub> O (5:1) | air               |                 | 0.80 <sup>T</sup> |                |                            | CP/Ac-14 | A = DPBF; $\lambda_{\text{exc}} = 434$ nm.   | 88F582 |
| <b>1.52 9,10-Anthraquinone, 1,8-diamino-</b>   |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.35 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air               |                 | 0.77 <sup>T</sup> |                |                            | CP/Pa-14 | A = DMA; P = 9,10-Dimethylanthracene endoperoxide; $\lambda_{\text{exc}} = 435$ nm. $P_T^{O_2} = 1$ .  | 80E446 |
|  | 2-PrOH/H <sub>2</sub> O (5:1) | air               |                 | 0.58 <sup>T</sup> |                |                            | CP/Ac-43 | $S' = 1,5\text{-AQ(NH}_2\text{)}_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 545$ nm.                          | 88F582 |
| <b>1.53 9,10-Anthraquinone, 2,6-diamino-</b>   |                               |                   |                 |                   |                |                            |          |  |        |
|  | 2-PrOH/H <sub>2</sub> O (5:1) | air               |                 | 0.05 <sup>T</sup> |                |                            | CP/Ac-43 | $S' = 1,5\text{-AQ(NH}_2\text{)}_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 434$ nm.                          | 88F582 |
| <b>1.54 9,10-Anthraquinone, 1,5-diamino-2-bromo-4,8-dihydroxy-</b>                     |                               |                   |                 |                   |                |                            |          |  |        |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.35 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | CHCl <sub>3</sub>             | air <sup>a</sup>  |                 | 0.15 <sup>T</sup> |                |                            | PL/LI-56 | $S' = \text{MPDEE}$ ; rel. to $\phi_{\Delta}(S') = 0.77$ . $P_T^{O_2} = 1$ .   | 82F631 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                           | [O <sub>2</sub> ]   | $\phi_{\Delta}$ | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|--|-----------------------------------|---------------------|-----------------|-------------------|----------------|----------------------------|-------------|--|--------|
| <b>1.54 9,10-Anthraquinone, 1,5-diamino-2-bromo-4,8-dihydroxy</b> —Continued   |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CCl <sub>4</sub>                  | air                 |                 | 0.20 <sup>T</sup> |                |                            | MP/LI-56    | $S' = \text{TPBC}$ ; rel. to $\phi_{\Delta}(S') = 0.45$ .  | 82A384 |
|  | EtOH                              | air <sup>a</sup>    |                 | 0.16 <sup>T</sup> |                |                            | CP/Oc-43    | $S' = \text{MPDEE}$ ; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to $\phi_{\Delta}(S') = 0.77$ . Assumed $P_T^{O_2} = 1$ , $P_S^{O_2} = 0$ . | 82F631 |
| <b>1.55 9,10-Anthraquinone, 1,5-diamino-4,8-dihydroxy</b>                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.38 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.56 9,10-Anthraquinone, 1,8-diamino-4,5-dihydroxy</b>                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.58 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
|  | EtOH                              | air                 |                 | 0.28 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
|  | MeOH                              | air                 |                 | 0.18 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
| <b>1.57 9,10-Anthraquinone, 2,5-diamino-1,8-dihydroxy</b>                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | EtOH                              | air                 |                 | 0.12 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
|  | MeOH                              | air                 |                 | 0.08 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
| <b>1.58 9,10-Anthraquinone, 2,7-diamino-1,8-dihydroxy</b>                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | EtOH                              | air                 |                 | 0.08 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
|  | MeOH                              | air                 |                 | 0.07 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 91F197 |
| <b>1.59 9,10-Anthraquinone, 1,4-diamino-2-methoxy</b>                          |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.01 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$   | 86E640 |
|  | 2-PrOH/<br>H <sub>2</sub> O (5:1) | air                 |                 | 0.05 <sup>T</sup> |                |                            | CP/Ac-43    | $S' = 1,5\text{-AQ(NH}_2)_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 545$ nm.                                 | 88F582 |
| <b>1.60 9,10-Anthraquinone, 1,4-diamino-2-[4-(phenylaminosulfonyl)phenoxy]</b> |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.01 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.61 9,10-Anthraquinone, 1,2-dihydroxy</b>                                  |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.01 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.62 9,10-Anthraquinone, 1,8-dihydroxy</b>                                  |                                   |                     |                 |                   |                |                            |             |  |        |
|  | C <sub>5</sub> H <sub>5</sub> N   | O <sub>2</sub> var. |                 | 0.84 <sup>T</sup> |                |                            | CP/Oc-14    | A = $\alpha$ -Terpinene.   | 587004 |
|  | CH <sub>3</sub> CN                | air                 |                 | 0.70 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 90D185 |
|  | DMSO                              | air                 |                 | 0                 |                |                            | CP/LI-56    | $S' = \text{RB}$ . No detectable phosphorescence.  | 90D185 |
|  | EtOH                              | air                 |                 | 0.43 <sup>T</sup> |                |                            | CP/LI-56    | $S' = \text{RB}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 90D185 |
| <b>1.63 9,10-Anthraquinone, 1-hydroxy</b>                                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.2 <sup>T</sup>  |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.64 9,10-Anthraquinone, 2-hydroxy</b>                                      |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.03 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.77^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.65 9,10-Anthraquinone, 1,4,5,8-tetraamino</b>                             |                                   |                     |                 |                   |                |                            |             |  |        |
|  | 2-PrOH/<br>H <sub>2</sub> O (5:1) | air                 |                 | 0.10 <sup>T</sup> |                |                            | CP/Ac-43    | $S' = 1,5\text{-AQ(NH}_2)_2$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.80$ ; $\lambda_{\text{exc}} = 545$ nm.                                 | 88F582 |
| <b>1.66 9,10-Anthraquinone, 1,4,5,8-tetrahydroxy</b>                           |                                   |                     |                 |                   |                |                            |             |  |        |
|  | CHCl <sub>3</sub>                 | air <sup>a</sup>    |                 | 0.92 <sup>T</sup> |                |                            | PL/LI-56    | $S' = \text{MPDME}$ ; rel. to $\phi_{\Delta}(S') = 0.80^b$ . $P_T^{O_2} = 1$ .   | 86E640 |
| <b>1.67 Anthrone</b>   |                                   |                     |                 |                   |                |                            |             |  |        |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>      |                 | 0.25 <sup>T</sup> | 0.25           |                            | PL/LI-56,42 | $S' = \text{Pz}$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 1$ . Measured $P_T^{O_2} = 1$ .                                      | 88E449 |
|  | C <sub>6</sub> H <sub>6</sub>     | O <sub>2</sub>      |                 | 0.25 <sup>T</sup> | 0.25           |                            | PL/Hp-52,42 | $\lambda_{\text{exc}} = 355$ nm; used $\phi_T(S) = 1$ . Measured $\phi_{\Delta} = 0.25$ , $P_T^{O_2} = 1$ and $\phi_F$ .                       | 88E449 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]       | ϕ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.   |
|---|---|-------------------------|-------------------|-----------------------------|-----------------------------|----------------------|-------------|---|--------|
| <b>1.68 Anthrone, 1,8-dihydroxy- (Anthralin)</b>                                      |   |                         |                   |                             |                             |                      |             |   |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                     | <0.01             |                             |                             |                      | PL/LI-56    | S' = Np; rel. to ϕ <sub>Δ</sub> (S') ~ 0.55; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> > 0.94; no detectable luminescence.   | 89E158 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                     |                   | 0.77*                       | 0.64                        |                      | PR/βCb-59   | S' = BP; TA = Car; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.29; used ε <sub>T</sub> (S) = 4770 L mol <sup>-1</sup> cm <sup>-1</sup> at 560 nm, ε <sub>T</sub> (S') = 7630 L mol <sup>-1</sup> cm <sup>-1</sup> at 532.5 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> > 0.94.                           | 89E158 |
|   | DMSO  | air                     | 0                 |                             |                             |                      | CP/LI-56    | S' = RB. No detectable phosphorescence.   | 90D185 |
|   | EtOH  | air                     | 0                 |                             |                             |                      | CP/LI-56    | S' = RB. No detectable phosphorescence.   | 90D185 |
|   | CH <sub>3</sub> CN                            | air                     | 0                 |                             |                             |                      | CP/LI-56    | S' = RB. HCl added; no detectable phosphorescence.  | 90D185 |
| <b>1.69 Anthrone, 1,8-dihydroxy-, conjugate base</b>                                  |   |                         |                   |                             |                             |                      |             |   |        |
|   | CH <sub>3</sub> CN                            | air                     | ≥0.11             |                             |                             |                      | CP/LI-56    | S' = RB; rel. to ϕ <sub>Δ</sub> (S') = 0.80 <sup>b</sup> . 15% quenching of singlet oxygen by S.  | 90D185 |
| <b>1.70 Azulene</b>   |   |                         |                   |                             |                             |                      |             |   |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>        |                   | 0                           | 0                           |                      | CP/Ac-14,38 | λ <sub>exc</sub> = 546.1 nm. A = DMA and DMBA.  | 69F388 |
| <b>1.71 Benzaldehyde</b>  |   |                         |                   |                             |                             |                      |             |   |        |
|   | MeOH  | O <sub>2</sub>          | 0.61              |                             |                             |                      | CP/Oc-14    | A = TME; λ <sub>exc</sub> = 283-373 nm.   | 70F735 |
|   | MeOH  | O <sub>2</sub>          | <0.58             |                             |                             |                      | CP/Oc-14    | A = 2,5-DMF; λ <sub>exc</sub> = 283-373 nm. Some free radical reaction occurs.  | 70F735 |
| <b>1.72 Benz[a]anthracene</b>   |   |                         |                   |                             |                             |                      |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.2 × 10 <sup>-3</sup>  |                   |                             | 0.95                        |                      | PL/Ad,St-48 | A = Rub; meas. ϕ <sub>T</sub> (S) = 0.85; λ <sub>exc</sub> = 347 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 1; used ε <sub>T</sub> (S) = 15,000 L mol <sup>-1</sup> cm <sup>-1</sup> at λ <sub>max</sub> ; n <sub>Δ</sub> = 0.95.  | 83F075 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.2 × 10 <sup>-3</sup>  | 1.4               |                             |                             |                      | PL/LI-56    | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 82E010 |
|   | C <sub>6</sub> H <sub>5</sub> CN              | 1.2 × 10 <sup>-3</sup>  |                   |                             | 0.21                        |                      | PL/Ad,St-48 | A = Rub; meas. ϕ <sub>T</sub> (S) = 0.75; λ <sub>exc</sub> = 347 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 1; used ε <sub>T</sub> (S) = 12,000 L mol <sup>-1</sup> cm <sup>-1</sup> at λ <sub>max</sub> ; n <sub>Δ</sub> = 0.21.  | 83F075 |
| <b>1.73 Benz[a]anthracene, 9,10-dimethyl-</b>   |   |                         |                   |                             |                             |                      |             |   |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>        | 0.69 <sup>T</sup> | 1.0                         |                             | 1.0                  | CP/Ac-14,40 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> from ϕ <sub>Δ</sub> when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 1; ϕ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> = ϕ <sub>Δ</sub> when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. | 767422 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>        |                   |                             | ≤0.34                       | ≤1.3                 | CP/Ac-14,38 | A = S. Assumed f <sub>Δ</sub> <sup>T</sup> = 1 and f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 76F905 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub> var.     |                   |                             |                             |                      | CP/Ac-14,38 | A = S; λ <sub>exc</sub> = 365 nm. ϕ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> / (f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> ) = 0.66.   | 68F286 |
| <b>1.74 Benzene, 5-chloro-1,3-dimethoxy-</b>  |   |                         |                   |                             |                             |                      |             |   |        |
|   | D <sub>2</sub> O                              | air                     | 0.0092            |                             |                             |                      | PL/LI-56    | S' = RB; rel. to ϕ <sub>Δ</sub> (S') = 0.78; λ <sub>exc</sub> = 308 nm.   | 91A341 |
| <b>1.75 Benzene, 1,3,5-triphenyl-</b>   |   |                         |                   |                             |                             |                      |             |   |        |
|   | n-C <sub>6</sub> H <sub>14</sub>              | air                     | 0.4 <sup>T</sup>  |                             |                             |                      | PL/Ad-43    | S' = An; A = DPBF; rel. to ϕ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 264 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 82E258 |
| <b>1.76 Benzenebutanoic acid, α-amino-2-(formylamino)-γ-oxo- (N-Formylkynurenone)</b> |   |                         |                   |                             |                             |                      |             |   |        |
|   | H <sub>2</sub> O pH = 7.4                     | air                     | 0.17              |                             |                             |                      | CP/Pa-43    | S' = RB; A = Im; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 332 nm. RNO as monitor of P.  | 91R141 |
|   | H <sub>2</sub> O pH = 7.5                     | 0.15 × 10 <sup>-3</sup> | 0.15              | 0.75                        |                             |                      | CP/Ac-14,42 | A = TrpH; meas. ϕ <sub>T</sub> (S) = 0.20 <sup>f</sup> ; λ <sub>exc</sub> = >320 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; with k <sub>d</sub> = k <sub>Δ</sub> + k <sub>S</sub> [S].  | 78A358 |
|   | H <sub>2</sub> O pH = 7.5                     | 2 × 10 <sup>-3</sup>    | 0.17              | 0.85                        |                             |                      | CP/Ac-14,42 | A = TrpH; meas. ϕ <sub>T</sub> (S) = 0.20 <sup>f</sup> ; λ <sub>exc</sub> = >320 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; in presence of Type I photooxidation; with k <sub>d</sub> = k <sub>Δ</sub> + k <sub>S</sub> [S].  | 78A358 |
| <b>1.77 Benzenebutanoic acid, α,2-diamino-3-hydroxy-γ-oxo- (3-Hydroxykynurenone)</b>  |   |                         |                   |                             |                             |                      |             |   |        |
|   | D <sub>2</sub> O pD = 7                       | air                     | 0.003             |                             |                             |                      | PL/LI-56    | S' = RF; rel. to ϕ <sub>Δ</sub> (S') = 0.30; λ <sub>exc</sub> = 337 nm.   | 87F290 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ]     | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.   |
|--|---|-----------------------|-------------------|----------------|----------------|----------------------------|-------------|---|--------|
| <b>1.77 Benzenebutanoic acid, <math>\alpha</math>,2-diamino-3-hydroxy-<math>\gamma</math>-oxo- (3-Hydroxykynurenone)—Continued</b> |   |                       |                   |                |                |                            |             |   |        |
|  | H <sub>2</sub> O<br>pH = 7.4                  | air                   | 0                 |                |                |                            | CP/Pa-43    | $S' = RB$ ; A = Im; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 360$ nm. RNO as monitor of P.   | 91R141 |
| <b>1.78 Benzenebutanoic acid, <math>\alpha</math>,2-diamino-<math>\gamma</math>-oxo- (Kynurenone)</b>                              |   |                       |                   |                |                |                            |             |   |        |
|  | D <sub>2</sub> O pD = 7                       | air                   | 0.006             |                |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.30$ .  | 87F290 |
|  | H <sub>2</sub> O<br>pH = 7.4                  | air                   | 0                 |                |                |                            | CP/Pa-43    | $S' = RB$ ; A = Im; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 360$ nm. RNO as monitor of P.   | 91R141 |
| <b>1.79 1,3-Benzenediol (Resorcinol)</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | diox  | air                   | 0.12              |                |                |                            | PL/LI-56    | $S' = ZnTPP$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; $\lambda_{exc} = 308$ nm.   | 91A341 |
| <b>1.80 1,3-Benzenediol, 4-chloro-</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | diox  | O <sub>2</sub>        | 0.05              |                |                |                            | PL/LI-56    | $S' = ZnTPP$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; $\lambda_{exc} = 308$ nm.   | 91A341 |
| <b>1.81 1,4-Benzenediol (Hydroquinone)</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | diox  | air                   | 0.21              |                |                |                            | PL/LI-56    | $S' = ZnTPP$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; $\lambda_{exc} = 308$ nm. May be from quinone contaminants.   | 91A341 |
| <b>1.82 1,4-Benzenediol, chloro-</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | diox  | O <sub>2</sub>        | 0.04              |                |                |                            | PL/LI-56    | $S' = ZnTPP$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; $\lambda_{exc} = 308$ nm. May be from quinone contaminants.   | 91A341 |
| <b>1.83 Benzil</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.57              | 0.62           |                |                            | CP/Pa-14.42 | A = 1,2-Dimethylcyclohexene: $\lambda_{exc} = 366$ nm; used $\phi_T(S) = 0.92^d$ . P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenedecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene. | 85F153 |
| <b>1.84 Benzil, 4,4'-dichloro-</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.23              |                |                |                            | CP/Pa-14    | A = 1,2-Dimethylcyclohexene; $\lambda_{exc} = 366$ nm. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenedecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene.                             | 85F153 |
| <b>1.85 Benzil, 4,4'-dimethoxy-</b>  |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.27              |                |                |                            | CP/Pa-14    | A = 1,2-Dimethylcyclohexene; $\lambda_{exc} = 366$ nm. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenedecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene.                             | 85F153 |
| <b>1.86 Benzil, 2,2',4,4',6,6'-hexamethyl-</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.06              |                |                |                            | CP/Pa-14    | A = 1,2-Dimethylcyclohexene; $\lambda_{exc} = 366$ nm. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenedecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene.                             | 85F153 |
| <b>1.87 Benzo[1,2,3-kl:4,5,6-k'l']dixanthene (BDX)</b>   |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air                   |                   |                | 1.9            |                            | CP/Ac-14,38 | A = S. Assumed $f_T^{O_2} = 1$ , $\phi_{\Delta}^{f_T^T} = 0.08$ .   | 84F197 |
| <b>1.88 Benzophenone (BP)</b>  |   |                       |                   |                |                |                            |             |   |        |
|  | C <sub>6</sub> D <sub>6</sub>                 | air                   | 0.29 <sup>T</sup> | 0.29           |                |                            | PL/LI-56,42 | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 1$ . S' = BP in benzene, used $\phi_{\Delta}(S')$ in benzene = 0.29.  | 88E657 |
|  | C <sub>6</sub> H <sub>6</sub>                 | air or O <sub>2</sub> | 0.35              | 0.35           |                |                            |             | See Table 4.  |        |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                  | [O <sub>2</sub> ] | Φ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method          | Comment  | Ref.   |
|--|--------------------------|-------------------|-------------------|-----------------------------|-----------------------------|----------------------|-----------------|--|--------|
| <b>1.88 Benzophenone (BP)—Continued</b>            |                          |                   |                   |                             |                             |                      |                 |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | air                      |                   | 0.36 <sup>T</sup> | ~0.37                       |                             |                      | PL/Hp-52,42     | λ <sub>exc</sub> = 337 nm. Measured Φ <sub>T</sub> , assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 91F198 |
| C <sub>6</sub> H <sub>6</sub>                      | air                      |                   | 0.31 <sup>T</sup> | 0.31                        |                             |                      | PL/LI-57,42     | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83; used Φ <sub>T</sub> (S) = 1.0. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 90A328 |
| C <sub>6</sub> H <sub>6</sub>                      | air                      |                   | 0.33*             | 0.29 <sup>T</sup>           | 0.29                        |                      | PL/LI-60,42     | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55; λ <sub>exc</sub> = 355 nm; used Φ <sub>T</sub> (S) = 1 <sup>c</sup> .  | 87E234 |
| C <sub>6</sub> H <sub>6</sub>                      | air                      |                   | 0.29 <sup>T</sup> | 0.29                        |                             |                      | PL/LI,St-55,42  | S' = Ac; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm; used Φ <sub>T</sub> (S) = 1 <sup>c</sup> ; ε <sub>T</sub> (S) = 7630 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. Used ε <sub>T</sub> (S') = 24,300 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm, P <sub>T</sub> <sup>O<sub>2</sub></sup> (S) = 0.96, P <sub>T</sub> <sup>O<sub>2</sub></sup> (S') = 1. | 84E373 |
| C <sub>6</sub> H <sub>6</sub>                      | 1.9 × 10 <sup>-3</sup>   |                   | 0.54              |                             |                             |                      | CP/Ac-46        | A = DMA; λ <sub>exc</sub> = 365 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 1.1, 1.6 and 1.8 for S' = DMA, Rub and DPBF, resp.; solvent may contain impurities.   | 81F364 |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.35 <sup>T</sup> | 0.35                        |                             |                      | PL/Hp-52,42     | λ <sub>exc</sub> = 355 nm; used Φ <sub>T</sub> (S) = 1. Measured Φ <sub>Δ</sub> = 0.35, P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 and Φ <sub>F</sub> .   | 88E449 |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.35 <sup>T</sup> | 0.35                        |                             |                      | PL/LI-56,42     | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83; used Φ <sub>T</sub> (S) = 1. Measured P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E449 |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.39 <sup>T</sup> | 0.39                        |                             |                      | PL/Ad-49,42     | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.  | 84F005 |
| C <sub>6</sub> H <sub>6</sub>                      | 9.0 × 10 <sup>-3</sup>   |                   | 0.90              | 1                           | 0                           |                      | CP/Ac-46        | A = DMA; λ <sub>exc</sub> = 365 nm; used Φ <sub>T</sub> (S) = 1.0. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.90, 1.0 and 1.13 for S' = DMA, Rub and DPBF, resp.; solvent may contain impurities.  | 81F364 |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.4 <sup>T</sup>  | 0.4                         |                             |                      | PR/Ad,St-49,42  | A = DPBF; used Φ <sub>T</sub> (S) = 1.0, ε <sub>T</sub> (S) = 7630 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. Measured G( <sup>3</sup> S*).   | 78E263 |
| CDCl <sub>3</sub>                                  | ~1.16 × 10 <sup>-2</sup> |                   | 0.55 <sup>T</sup> | 0.55                        |                             |                      | PL/Ad,St-49,42  | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used Φ <sub>T</sub> (S) = 1 <sup>f</sup> , ε <sub>T</sub> (S) = 7640 L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. P <sub>A</sub> = 1.  | 87E410 |
| CH <sub>3</sub> CN                                 | O <sub>2</sub>           |                   | 0.37 <sup>T</sup> | 0.37                        |                             |                      | PL/Ad,St-49,42  | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 2.5 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 1.0 × 10 <sup>9</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (S) = 1 <sup>d</sup> , ε <sub>T</sub> (AC) = 6500 L mol <sup>-1</sup> cm <sup>-1</sup> at 520 nm. Showed P <sub>T</sub> <sup>O<sub>2</sub></sup> (S and S') > 0.95.                       | 85A268 |
| MeOH   | O <sub>2</sub>           |                   | <0.50             |                             |                             |                      | CP/Oc-14        | A = 2,5-DMF; λ <sub>exc</sub> = 283-373 nm. Some free radical reaction occurs.   | 70F735 |
| <b>1.89 Benzophenone, 4,4'-bis(dimethylamino)-</b> |                          |                   |                   |                             |                             |                      |                 |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.37*             | 0.41 <sup>T</sup>           | 0.41                        |                      | PL/Ad,TAt-50,42 | S' = BP; A = DPBF; TA = 1-MeNp; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.39; meas. Φ <sub>T</sub> (S) = 1 <sup>c</sup> ; λ <sub>exc</sub> = 337 nm. Showed P <sub>T</sub> <sup>O<sub>2</sub></sup> (S and S') > 0.95.  | 85A268 |
| CH <sub>3</sub> CN                                 | O <sub>2</sub>           |                   | 0.16 <sup>T</sup> | 0.35                        |                             |                      | PL/Ad,TAt-50,42 | S' = BP; A = DPBF; TA = 1-MeNp; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.37; meas. Φ <sub>T</sub> (S) = 0.47 <sup>e</sup> ; λ <sub>exc</sub> = 337 nm. Showed P <sub>T</sub> <sup>O<sub>2</sub></sup> (S and S') > 0.95.   | 85A268 |
| <b>1.90 Benzophenone, 4,4'-dimethoxy-</b>          |                          |                   |                   |                             |                             |                      |                 |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>           |                   | 0.30*             | 0.34 <sup>T</sup>           | 0.34                        |                      | PL/Ad,TAt-50,42 | S' = BP; A = DPBF; TA = 1-MeNp; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.39; meas. Φ <sub>T</sub> (S) = 1 <sup>c</sup> ; λ <sub>exc</sub> = 337 nm. Showed P <sub>T</sub> <sup>O<sub>2</sub></sup> (S and S') > 0.95.  | 85A268 |
| CH <sub>3</sub> CN                                 | O <sub>2</sub>           |                   | 0.40 <sup>T</sup> | 0.40                        |                             |                      | PL/Ad,TAt-50,42 | S' = BP; A = DPBF; TA = 1-MeNp; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.37; meas. Φ <sub>T</sub> (S) = 1 <sup>c</sup> ; λ <sub>exc</sub> = 337 nm. Showed P <sub>T</sub> <sup>O<sub>2</sub></sup> (S and S') > 0.95.  | 85A268 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]            | $\phi_{\Delta}$   | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method          | Comment   | Ref.   |
|-------|--|------------------------------|-------------------|-------------------|----------------|----------------------------|-----------------|---|--------|
| 1.91  | Benzophenone, 4-fluoro-  |                              |                   |                   |                |                            |                 |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>               |                   | 0.39*             | 0.43           |                            | PL/Ad,TAt-50,42 | $S' = BP; A = DPBF; TA = 1\text{-MeNp}; \text{rel. to } f_{\Delta}^T(S') = 0.39; \text{meas. } \phi_T(S) = 1^e; \lambda_{\text{exc}} = 337 \text{ nm. Showed } P_T^{O_2} (S \text{ and } S') > 0.95.$ | 85A268 |
|       |  |                              | 0.43 <sup>T</sup> |                   |                |                            |                 |   |        |
|       | CH <sub>3</sub> CN   | O <sub>2</sub>               |                   | 0.44 <sup>T</sup> | 0.44           |                            | PL/Ad,TAt-50,42 | $S' = BP; A = DPBF; TA = 1\text{-MeNp}; \text{rel. to } f_{\Delta}^T(S') = 0.37; \text{meas. } \phi_T(S) = 1^e; \lambda_{\text{exc}} = 337 \text{ nm. Showed } P_T^{O_2} (S \text{ and } S') > 0.95.$ | 85A268 |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.92  | Benzophenone, 4-(trifluoromethyl)-   |                              |                   |                   |                |                            |                 |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>               |                   | 0.38*             | 0.42           |                            | PL/Ad,TAt-50,42 | $S' = BP; A = DPBF; TA = 1\text{-MeNp}; \text{rel. to } f_{\Delta}^T(S') = 0.39; \text{meas. } \phi_T(S) = 1^e; \lambda_{\text{exc}} = 337 \text{ nm. Showed } P_T^{O_2} (S \text{ and } S') > 0.95.$ | 85A268 |
|       |  |                              | 0.42 <sup>T</sup> |                   |                |                            |                 |   |        |
|       | CH <sub>3</sub> CN   | O <sub>2</sub>               |                   | 0.54 <sup>T</sup> | 0.54           |                            | PL/Ad,TAt-50,42 | $S' = BP; A = DPBF; TA = 1\text{-MeNp}; \text{rel. to } f_{\Delta}^T(S') = 0.37; \text{meas. } \phi_T(S) = 1^e; \lambda_{\text{exc}} = 337 \text{ nm. Showed } P_T^{O_2} (S \text{ and } S') > 0.95.$ | 85A268 |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.93  | Benzo[ <i>a</i> ]phenothiazine   |                              |                   |                   |                |                            |                 |   |        |
|       | CH <sub>3</sub> CN   | O <sub>2</sub>               |                   | ~0.2              |                |                            | PL/LI-56        | $S' = Pz; \text{rel. to } \phi_{\Delta}(S') = 0.83; \lambda_{\text{exc}} = 355 \text{ nm.}$   | 91A308 |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.94  | Benzo[ <i>b</i> ]phenothiazine   |                              |                   |                   |                |                            | PL/LI-56        | $S' = Pz; \text{rel. to } \phi_{\Delta}(S') = 0.83; \lambda_{\text{exc}} = 355 \text{ nm.}$   | 91A308 |
|       | CH <sub>3</sub> CN   | O <sub>2</sub>               |                   | 0.19              |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.95  | Benzo[ <i>c</i> ]phenothiazine   |                              |                   |                   |                |                            | PL/LI-56        | $S' = Pz; \text{rel. to } \phi_{\Delta}(S') = 0.83; \lambda_{\text{exc}} = 355 \text{ nm.}$   | 91A308 |
|       | CH <sub>3</sub> CN   | O <sub>2</sub>               |                   | 0.17              |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.96  | 1-Benzopyran-4-one, 2,3-diphenyl- (3-Phenylflavone)                              |                              |                   |                   |                |                            | PL/Ad-43,39     | $S' = BP; A = DPBF; \text{rel. to } \phi_{\Delta}(S') = 0.4; \text{meas. } \phi_T(S) = 0.5^f; \lambda_{\text{exc}} = 337 \text{ nm.}$   | 86E567 |
|       | C <sub>6</sub> H <sub>6</sub>  | (0.6-5.5) × 10 <sup>-3</sup> | 0.4 <sup>T</sup>  | 0.8               |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.97  | 1-Benzopyran-4-one, 3-hydroxy-2-phenyl- (3-Hydroxyflavone)                       |                              |                   |                   |                |                            | PL/LI-56        | $S' = Np; TD = DP; \text{rel. to } f_{\Delta}^T(S') = 1.0; \lambda_{\text{exc}} = 355 \text{ nm. } P_T^{O_2} = 1, \phi_{et} = 1.$   | 89E365 |
|       | <i>n</i> -C <sub>7</sub> H <sub>16</sub>   | 2.3 × 10 <sup>-3</sup>       | 0.18              |                   |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.98  | 1-Benzopyran-4-one, 2-phenyl- (Flavone)  |                              |                   |                   |                |                            | PL/Ad-43,39     | $S' = BP; A = DPBF; \text{rel. to } \phi_{\Delta}(S') = 0.4; \text{meas. } \phi_T(S) = 0.9^f; \lambda_{\text{exc}} = 337 \text{ nm.}$   | 86E567 |
|       | C <sub>6</sub> H <sub>6</sub>  | (0.6-5.5) × 10 <sup>-3</sup> | 0.5*              |                   |                |                            |                 |   |        |
|       |  |                              | 0.6 <sup>T</sup>  | 0.7               |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.99  | [1]Benzopyrano[6,7,8- <i>ij</i> ]quinolizin-11-one, 2,3,6,7-tetrahydro-9-methyl- |                              |                   |                   |                |                            | CP/Pa-14        | $A = Rub; \lambda_{\text{exc}} = 365 \text{ nm.}$   | 87F569 |
|       | C <sub>6</sub> H <sub>6</sub>  | air                          |                   | 0.08              |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.100 | 1,4-Benzoquinone, 2,6-diphenyl-  |                              |                   |                   |                |                            | PL/LI-56        | $S' = TPP; \text{rel. to } \phi_{\Delta}(S') = 0.82; \lambda_{\text{exc}} = 530 \text{ nm.}$  | 88E124 |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | O <sub>2</sub>               |                   | 1.1               |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.101 | 1,4-Benzoquinone, 2,6-diphenyl-, complex with Triphenylamine                     |                              |                   |                   |                |                            | PL/LI-56        | $S' = TPP; \text{rel. to } \phi_{\Delta}(S') = 0.82; \lambda_{\text{exc}} = 530 \text{ nm. } \text{Triplet ion-radical pair.}$  | 88E124 |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | O <sub>2</sub>               |                   | 0.14              |                |                            |                 |   |        |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.102 | 1,4-Benzoquinone, tetrachloro- (Chloranil)                                       |                              |                   |                   |                |                            | PL/LI-56,42     | $S' = BP; \text{rel. to } \phi_{\Delta}(S') = 0.30; \lambda_{\text{exc}} = 355 \text{ nm; used } \phi_T(S) = 1.$  | 91E444 |
|       | C <sub>6</sub> H <sub>6</sub>  | →∞                           |                   | 0.85*             |                |                            |                 |   |        |
|       |  |                              | 0.73 <sup>T</sup> | 0.73              |                |                            |                 |   |        |
|       | CHCl <sub>3</sub>  | →∞                           |                   | 0.75 <sup>T</sup> | 0.75           |                            | PL/LI-56,42     | $S' = BP; \text{rel. to } \phi_{\Delta}(S') = 0.30; \lambda_{\text{exc}} = 355 \text{ nm; used } \phi_T(S) = 1. \text{ rel. to } S' \text{ in benzene, cor. for solvent } k_T.$                       | 91E444 |
|       |  |                              |                   |                   |                |                            |                 |   |        |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | →∞                           |                   | 0.35 <sup>T</sup> | 0.35           |                            | PL/LI-56,42     | $S' = BP; \text{rel. to } \phi_{\Delta}(S') = 0.30; \lambda_{\text{exc}} = 355 \text{ nm; used } \phi_T(S) = 1. \text{ rel. to } S' \text{ in benzene, cor. for solvent } k_T.$                       | 91E444 |
|       |  |                              |                   |                   |                |                            |                 |   |        |
| 1.103 | 1,4-Benzoquinone, tetrachloro-, complex with Anisole                             |                              |                   |                   |                |                            | PL/LI-56,42     | $S' = BP; \text{rel. to } \phi_{\Delta}(S') = 0.30; \lambda_{\text{exc}} = 355 \text{ nm; used } \phi_T(S) = 1. \text{ Triplet ion-radical pair.}$  | 91E444 |
|       | C <sub>6</sub> H <sub>6</sub>  | →∞                           |                   | 0.06*             |                |                            |                 |   |        |
|       |  |                              | 0.05 <sup>T</sup> | 0.05              |                |                            |                 |   |        |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]      | Φ <sub>Δ</sub>     | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.             |
|-------|--|------------------------|--------------------|-----------------------------|-----------------------------|----------------------|-------------|---|------------------|
| 1.104 | 1,4-Benzoquinone, tetrachloro-, complex with Durene                              |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>6</sub>  | →∞                     | 0.22*              | 0.19 <sup>T</sup>           | 0.19                        |                      | PL/LI-56,42 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.30; λ <sub>exc</sub> = 355 nm; used ϕ <sub>T</sub> (S) = 1. Triplet ion-radical pair.  | 91E444           |
| 1.105 | 1,4-Benzoquinone, tetrachloro-, complex with Hexamethylbenzene                   |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>6</sub>  | →∞                     | 0.23*              | 0.20 <sup>T</sup>           | 0.20                        |                      | PL/LI-56,42 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.30; λ <sub>exc</sub> = 355 nm; used ϕ <sub>T</sub> (S) = 1. Triplet ion-radical pair.  | 91E444           |
| 1.106 | 1,4-Benzoquinone, tetrachloro-, complex with 1,2,3-Trimethoxybenzene             |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>6</sub>  | →∞                     | 0.09*              | 0.08 <sup>T</sup>           | 0.08                        |                      | PL/LI-56,42 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.30; λ <sub>exc</sub> = 355 nm; used ϕ <sub>T</sub> (S) = 1. Triplet ion-radical pair.  | 91E444           |
| 1.107 | 1,4-Benzoquinone, tetramethyl- (Duroquinone)                                     |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | 1.2 × 10 <sup>-3</sup> |                    |                             |                             | 1.0                  | PL/Ad,St-48 | A = Rub; meas. ϕ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 347 nm; used ε <sub>T</sub> (S) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 490 nm. n <sub>Δ</sub> = 1.0.  | 83F075           |
| 1.108 | Biacetyl   |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>         | 0.57 <sup>T</sup>  | 0.57                        |                             |                      | CP/Pa-14,42 | A = 1,2-Dimethylcyclohexene; λ <sub>exc</sub> = 366 nm; used ϕ <sub>T</sub> (S) = 1. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene. | 85F153           |
| 1.109 | Bicyclo[2.2.1]heptane-2,3-dione, 1,7,7-trimethyl- (Camphoroquinone, CQ)          |                        |                    |                             |                             |                      |             |   |                  |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>         | 0.84               |                             |                             |                      | CP/Pa-14    | A = 1,2-Dimethylcyclohexene; λ <sub>exc</sub> = 366 nm. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylidenecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene.                              | 85F153           |
| 1.110 | Bicyclo[2.2.1]heptane-2-thione (Thionorcamphor)                                  |                        |                    |                             |                             |                      |             |   |                  |
|       | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>   | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1. [S] → 0, Φ <sub>Δ</sub> = 0.56 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| 1.111 | Bicyclo[2.2.1]heptane-2-thione, 3,3-dimethyl- (Thiocamphenilone)                 |                        |                    |                             |                             |                      |             |   |                  |
|       | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>   | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1.0. [S] → 0, Φ <sub>Δ</sub> = 0.59 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| 1.112 | Bicyclo[2.2.1]heptane-2-thione, 1,3,3,7,7-pentamethyl- (3,3-Dimethylthiocamphor) |                        |                    |                             |                             |                      |             |   |                  |
|       | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>   | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1.0. [S] → 0, Φ <sub>Δ</sub> = 0.91 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| 1.113 | Bicyclo[2.2.1]heptane-2-thione, 1,3,3-trimethyl- (Thiofenchone)                  |                        |                    |                             |                             |                      |             |   |                  |
|       | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>   | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1.0. [S] → 0, Φ <sub>Δ</sub> = 0.83 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| 1.114 | Bicyclo[2.2.1]heptane-2-thione, 1,7,7-trimethyl- (Thiocamphor)                   |                        |                    |                             |                             |                      |             |   |                  |
|       | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>   | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1.0. [S] → 0, Φ <sub>Δ</sub> = 0.87 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| 1.115 | Biphenyl   |                        |                    |                             |                             |                      |             |   |                  |
|       | c-C <sub>6</sub> H <sub>12</sub>   | →∞                     | 0.73 <sup>ST</sup> |                             |                             |                      | PL/LI-56    | S' = Py; rel. to Φ <sub>Δ</sub> (S') = 0.81; λ <sub>exc</sub> = 355 nm.   | 91E297           |
|       | c-C <sub>6</sub> H <sub>12</sub>   | air                    |                    | 1.0                         |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm.   | 87E234           |
|       | C <sub>6</sub> H <sub>6</sub>  | air                    | 0.51*              | 0.45                        |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55; λ <sub>exc</sub> = 355 nm.  | 87E234           |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>         |                    | 0.6                         |                             |                      | PR/Ad,St-49 | A = DPBF; used ϕ <sub>T</sub> (S) = 0.81, ε <sub>T</sub> (S) = 27,100 L mol <sup>-1</sup> cm <sup>-1</sup> at 367 nm. Measured G( <sup>3</sup> S*).   | 78E263           |
|       | CH <sub>3</sub> CN   | →∞                     | 0.27 <sup>ST</sup> |                             |                             |                      | PL/LI-56    | S' = DCA; rel. to Φ <sub>Δ</sub> (S') = 2.0; λ <sub>exc</sub> = 355 nm.   | 91E297           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]    | $\phi_{\Delta}$ | $f_{\Delta}^T$     | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|---|---|----------------------|-----------------|--------------------|----------------|----------------------------|-------------|--|--------|
| <b>1.115 Biphenyl—Continued</b>   |   |                      |                 |                    |                |                            |             |  |        |
|   | CH <sub>3</sub> CN                            | air                  |                 | 1.0                |                |                            | PL/LI-60    | $S' = Np$ ; TD = p-MAP; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{exc} = 355$ nm.   | 87E234 |
|   | H <sub>2</sub> O (mic)                        | O <sub>2</sub>       |                 | 1.0                |                |                            | PL/LI-60    | $S' = Np$ ; TD = BP; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{exc} = 355$ nm.  | 87E234 |
| <b>1.116 Bis(2,2'-bipyridine)bis(cyano)ruthenium(II)</b>  |   |                      |                 |                    |                |                            |             |  |        |
|   | MeOH  | O <sub>2</sub>       |                 | 0.79 <sup>T</sup>  |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.117 Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthrolineosmium(II)</b>     |   |                      |                 |                    |                |                            |             |  |        |
|   | MeOH  | O <sub>2</sub>       |                 | 0.74 <sup>T</sup>  |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.118 Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthroline-ruthenium(II)</b> |   |                      |                 |                    |                |                            |             |  |        |
|   | MeOH  | O <sub>2</sub>       |                 | 0.82 <sup>T</sup>  |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.119 5-Bromo-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion</b>               |   |                      |                 |                    |                |                            |             |  |        |
|   | MeOH  | O <sub>2</sub>       |                 | 0.80 <sup>T</sup>  |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.120 Carbon sixty-atom molecule (Buckminsterfullerene)</b>                                  |   |                      |                 |                    |                |                            |             |  |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air                  |                 | 1.0 <sup>T</sup>   | 1.0            |                            | PL/Hp-53,42 | $\lambda_{exc} = 510$ nm; used $\phi_T(S) = 1$ .   | 91E368 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.92 <sup>T</sup>  |                |                            | PL/Hp-52    | $\lambda_{exc} = 530$ nm.  | 91E534 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.98 <sup>T</sup>  |                |                            | PL/Hp-52    | $\lambda_{exc} = 340$ nm.  | 91E534 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.96 <sup>T</sup>  |                |                            | PL/LI-56    | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.62$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$ .  | 91E003 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.76 <sup>T</sup>  |                |                            | PL/LI-56    | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.62$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 91E003 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.76 <sup>T</sup>  |                |                            | PL/LI-56    | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .   | 91E003 |
| <b>1.121 Carbon seventy-atom molecule</b>   |   |                      |                 |                    |                |                            |             |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                  |                 | 0.81 <sup>T</sup>  | -1             |                            | PL/LI-56,42 | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.62$ ; meas. $\phi_T(S) = 0.9$ ; $\lambda_{exc} = 355, 532$ nm.   | 91E594 |
| <b>1.122 <math>\beta</math>-apo-14'-Carotenol (<i>all-trans</i>-C<sub>22</sub> aldehyde)</b>    |   |                      |                 |                    |                |                            |             |  |        |
|   | c-C <sub>6</sub> H <sub>12</sub>              | air                  |                 |                    |                |                            | PL/Ad-49,39 | $A = DPBF$ ; $AC = S$ ; $\lambda_{exc} = 337$ nm; used $k_d = 5 \times 10^4$ s <sup>-1</sup> , $k_A = 3.4 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\varepsilon_T(AC) = 121000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 470 nm. $f_{\Delta}^T P_T^{O_2} + P_S^{O_2} f_{\Delta}^S / \phi_T^{O_2} = 1.4$ . | 85F041 |
|   | c-C <sub>6</sub> H <sub>12</sub>              | O <sub>2</sub>       |                 | 0.48 <sup>T</sup>  | -1             |                            | PL/Ad-49,42 | $A = DPBF$ ; $AC = BP$ ; $\lambda_{exc} = 337$ nm; used $k_d = 5.0 \times 10^4$ s <sup>-1</sup> , $k_A = 3.4 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\phi_T(S) = 0.54^f$ , $\phi_T(AC) = 1$ , $\varepsilon_T(AC) = 7600$ L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.                               | 84F005 |
| <b>1.123 5-Chloro-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion</b>              |   |                      |                 |                    |                |                            |             |  |        |
|   | MeOH  | O <sub>2</sub>       |                 | 0.81 <sup>T</sup>  |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.124 Chrysene</b>   |   |                      |                 |                    |                |                            |             |  |        |
|   | c-C <sub>6</sub> H <sub>12</sub>              | $\rightarrow \infty$ |                 | 0.65 <sup>ST</sup> |                |                            | PL/LI-56    | $S' = Py$ ; rel. to $\phi_{\Delta}(S') = 0.81$ ; $\lambda_{exc} = 355$ nm.   | 91E297 |
|   | n-C <sub>6</sub> H <sub>14</sub>              | air                  |                 | 0.3                |                |                            | PL/Ad-43    | $S' = An$ ; $A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 264$ nm. $P_T^{O_2} = 1$ .   | 82E258 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | $1.2 \times 10^{-3}$ |                 | 1.2                |                |                            | PL/LI-56    | $S' = PdMPDME$ ; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.   | 82E010 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>       |                 | 0.66               |                |                            | PL/LI-56    | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ . Measured $P_T^{O_2} = 0.99$ and $\phi_T^{O_2} = \phi_T(S)$ . Authors assume $f_{\Delta}^S = 0$ and $\phi_T(S) = 0.81$ to give $f_{\Delta}^T = 0.81$ but $P_S^{O_2}$ is estimated to be >0.8 so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable.    | 88E449 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                    | [O <sub>2</sub> ] | $\phi_{\Delta}$    | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|--|----------------------------|-------------------|--------------------|----------------|----------------|----------------------------|-------------|--|--------|
| <b>1.124 Chrysene—Continued</b>                    |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | O <sub>2</sub>             |                   | 0.69               |                |                |                            | PL/Hp-52    | $\lambda_{exc} = 355$ nm. Measured $\phi_{\Delta} = 0.68$ , $P_T^{O_2} = 0.99$ and $\phi_T^{O_2} = \phi_T(S)$ and $\phi_F$ . Authors assume $f_{\Delta}^S = 0$ and $\phi_T(S) = 0.81$ to give $f_{\Delta}^T = 0.85$ but $P_S^{O_2}$ is estimated to be >0.8 so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable. | 88E449 |
| CCl <sub>4</sub>                                   | air                        |                   | 0.2                |                |                |                            | MP/LI-56    | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 652$ nm.   | 83E813 |
| CH <sub>3</sub> CN                                 | → ∞                        |                   | 0.30 <sup>ST</sup> |                |                |                            | PL/LI-56    | $S' = DCA$ ; rel. to $\phi_{\Delta}(S') = 2.0$ ; $\lambda_{exc} = 355$ nm.   | 91E297 |
| EtOH   | O <sub>2</sub>             |                   | 0.90               |                |                |                            | CP/Ac-43    | $S' = MB^+$ ; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.50^b$ ; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ .  | 74F648 |
| <b>1.125 Chrysene, 2-bromo-</b>                    |                            |                   |                    |                |                |                            |             |  |        |
| EtOH   | O <sub>2</sub>             |                   | 1                  |                |                |                            | CP/Ac-43    | $S' = MB^+$ ; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.50^b$ ; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ .  | 74F648 |
| <b>1.126 Chrysene, 2-chloro-</b>                   |                            |                   |                    |                |                |                            |             |  |        |
| EtOH   | O <sub>2</sub>             |                   | 1                  |                |                |                            | CP/Ac-43    | $S' = MB^+$ ; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.50^b$ ; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ .  | 74F648 |
| <b>1.127 Coronene</b>                              |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>      | $1.2 \times 10^{-3}$       |                   | 0.90               |                |                |                            | PL/LI-56    | $S' = PdMPDME$ ; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.   | 82E010 |
| C <sub>6</sub> H <sub>6</sub>                      | $1.9 \times 10^{-3}$       |                   | 0.94               |                |                |                            | CP/Ac-46    | $\lambda_{exc} = 365$ nm. Assumed $f_T^{O_2} = 1$ ; measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 1.80$ and 3.3 for $S' = A = DMA$ and DPBF, resp.  | 81F364 |
| C <sub>6</sub> H <sub>6</sub>                      | $9.0 \times 10^{-3}$       | 0.97              | ≥0.95              | 0              |                |                            | CP/Ac-46    | $\lambda_{exc} = 365$ nm; used $\phi_T(S) = 0.56$ . Assumed $f_T^{O_2} = 1$ ; measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.95$ and 1.25 for $S' = A = DMA$ and DPBF, resp.   | 81F364 |
| <b>1.128 Coumarin</b>                              |                            |                   |                    |                |                |                            |             |  |        |
| D <sub>2</sub> O                                   | air <sup>a</sup>           |                   | 0.01               |                |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.3$ ; $\lambda_{exc} = 337$ nm.  | 86F144 |
| MeOH   | air <sup>a</sup>           |                   | 0.03               |                |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.4$ ; $\lambda_{exc} = 337$ nm.  | 86F144 |
| <b>1.129 Coumarin, 7-(diethylamino)-4-methyl-</b>  |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | air                        |                   | 0.08               |                |                |                            | CP/Pa-14    | A = Rub; $\lambda_{exc} = 365$ nm.   | 87F569 |
| <b>1.130 Cycloheptatriene</b>                      |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | $2 \times 10^{-3}$         |                   | 0.80*              |                |                |                            | PL/LI-60    | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm. Measured $P_T^{O_2}$ .   | 89A235 |
|  |                            |                   | 0.66               |                |                |                            |             |  |        |
| <b>1.131 1,3-Cyclohexadiene</b>                    |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | $8.7 \times 10^{-4}$       |                   | 0.48*              |                |                |                            | PL/LI-60    | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm. Measured $P_T^{O_2}$ .   | 89A235 |
|  |                            |                   | 0.40               |                |                |                            |             |  |        |
| <b>1.132 2-Cyclohexenethione, 3,5,5-trimethyl-</b> |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | $(1.9-9.1) \times 10^{-3}$ | 0.9 <sup>T</sup>  | 0.9                |                |                |                            | PL/Ad-43,39 | $S' = DMTBP$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 1$ ; meas. $\phi_T(S) = 1$ ; $\lambda_{exc} = 532$ nm. Used $P_S^{O_2} = 0$ , $P_T^{O_2} = 1$ .  | 86A240 |
|  |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | $(1.9-9.1) \times 10^{-3}$ | 0.5*              | 0.6 <sup>T</sup>   | 0.6            |                |                            | PL/Ad-43,39 | $S' = BP$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.4$ ; meas. $\phi_T(S) = 1$ ; $\lambda_{exc} = 337$ nm. Used $P_S^{O_2} = 0$ , $P_T^{O_2} = 1$ .   | 86A240 |
|  |                            |                   |                    |                |                |                            |             |  |        |
| <b>1.133 Cyclopentadiene</b>                       |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | $8.7 \times 10^{-4}$       |                   | 0.90*              |                |                |                            | PL/LI-60    | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm. Measured $P_T^{O_2}$ .   | 89A235 |
|  |                            |                   | 0.75               |                |                |                            |             |  |        |
| <b>1.134 7-Dehydrocholesterol</b>                  |                            |                   |                    |                |                |                            |             |  |        |
| C <sub>6</sub> H <sub>6</sub>                      | air                        |                   | 0.96*              |                |                |                            | PL/LI-60    | $S' = Np$ ; TD = p-MAP; rel. to $f_{\Delta}^T(S') = 0.55$ ; $\lambda_{exc} = 355$ nm.  | 88E575 |
|  |                            |                   | 0.85               |                |                |                            |             |  |        |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]        | $\phi_{\Delta}$ | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.   |
|--|--|--------------------------|-----------------|-------------------|----------------|----------------------------|-------------|---|--------|
| <b>1.135 Diacenaphtho[1,2-<i>b</i>:2',1'-<i>d</i>]thiophene (DNT)</b>                    |  |                          |                 |                   |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                              | air <sup>a</sup>         |                 | 0.46              |                |                            | PL/LI-56    | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ . Supersedes 0.98 quoted in [83F172].  | 92F013 |
|  | CH <sub>3</sub> CN   | air <sup>a</sup>         |                 | 0.39              |                |                            | PL/LI-56    | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ . Supersedes 0.62 quoted in [83F172].  | 92F013 |
| <b>1.136 2,7-Diazapyrene, 2,7-dimethyl-</b>  |  |                          |                 |                   |                |                            |             |   |        |
|  | D <sub>2</sub> O   | O <sub>2</sub>           |                 | 0.14              |                |                            | PL/LI-56    | $S' = ZnTMpyP^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.88$ ; meas. $\phi_T(S) = 0.17$ ; $\lambda_{exc} = 355$ nm.   | 91R201 |
| <b>1.137 Dibenz[<i>a,h</i>]anthracene</b>  |  |                          |                 |                   |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>              | 1.2 × 10 <sup>-3</sup>   |                 |                   | 1.0            |                            | PL/Ad/St-48 | $A = Rub$ ; meas. $\phi_T(S) = 0.9$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ ; used $\epsilon_T(S) = 13,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at $\lambda_{max}$ ; $n_{\Delta} = 1.0$ .            | 83F075 |
|  | C <sub>6</sub> H <sub>5</sub> CN                           | 1.2 × 10 <sup>-3</sup>   |                 |                   | 0.23           |                            | PL/Ad/St-48 | $A = Rub$ ; meas. $\phi_T(S) = 0.9$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ ; used $\epsilon_T(S) = 10,500$ L mol <sup>-1</sup> cm <sup>-1</sup> at $\lambda_{max}$ ; $n_{\Delta} = 0.23$ .           | 83F075 |
| <b>1.138 Dibenzo[<i>def,mno</i>]chrysene (Anthanthrene)</b>                              |  |                          |                 |                   |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                              | O <sub>2</sub> var.      |                 | 1                 |                |                            | CP/Ac-14,38 | $\lambda_{exc} = 435.8$ nm. A = DMA and DMBA; results consistent with $f_{\Delta}^S \ll f_{\Delta}^T$ ; assumed $P_T^{O_2} = 1$ ; measured $\phi_T f_{\Delta}^T / (f_{\Delta}^T + f_{\Delta}^S) = 0.22$ . | 69F388 |
| <b>1.139 Dibenzo[<i>a,o</i>]perylene, 7,16-diphenyl- (Mesodiphenylhelianthrene. MDH)</b> |  |                          |                 |                   |                |                            |             |   |        |
|  | c-C <sub>6</sub> H <sub>12</sub>                           | air                      |                 | 0.33              |                |                            | CP/Ac-14    | $A = S$ ; $\lambda_{exc} = 578$ nm. Recalculated using $f_r^A = 0.30$ .   | 83F406 |
|  | n-C <sub>5</sub> H <sub>12</sub>                           | air                      |                 | 0.28              |                |                            | CP/Ac-A.18  | $A = S$ ; $\lambda_{exc} = 546$ nm. $f_r^A = 0.30$  | 87F480 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>              | air                      |                 | 0.67              |                |                            | CP/Ac-14,38 | $A = S$ ; meas. $\phi_T(S) = 0.52$ ; $\lambda_{exc} = 578$ nm. $f_T^{O_2} = 1$ , $f_r^A = 0.30$ , [O <sub>2</sub> ] varied, ( $f_{\Delta}^S + f_{\Delta}^T f_T^{O_2}$ ) = 1.2.                            | 87F479 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>              | (2-9) × 10 <sup>-3</sup> |                 |                   | 0.35           |                            | CP/Ac-14,38 | $A = S$ . Assumed $f_T^{O_2} = 1$ , $\phi_T f_{\Delta}^T = 0.16$ .  | 84F197 |
|  | CCl <sub>4</sub>   | air                      |                 | 0.50              |                |                            | CP/Ac-14    | $A = S$ . $f_T^{O_2} = 1$ , $f_r^A = 0.30$ , [O <sub>2</sub> ] varied.  | 87F479 |
|  | CH <sub>3</sub> COCH <sub>3</sub>                          | air                      |                 | 0.67              |                |                            | CP/Ac-A.18  | $A = S$ ; $\lambda_{exc} = 546$ nm. $f_r^A = 0.30$  | 87F480 |
|  | CHCl <sub>3</sub>  | air                      |                 | 0.43              |                |                            | CP/Ac-14    | $A = S$ ; $\lambda_{exc} = 578$ nm. Recalculated using $f_r^A = 0.30$ .   | 83F406 |
|  | CS <sub>2</sub>  | air                      |                 | 0.33              |                |                            | CP/Ac-14    | $A = S$ ; $\lambda_{exc} = 578$ nm. Recalculated using $f_r^A = 0.30$ .   | 83F406 |
|  | MeOH /C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> (97:3) | air                      |                 | 0.50              |                |                            | CP/Ac-A.18  | $A = S$ ; $\lambda_{exc} = 546$ nm. $f_r^A = 0.30$  | 87F480 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH           | air                      |                 | 0.43              |                |                            | CP/Ac-A.18  | $A = S$ ; $\lambda_{exc} = 546$ nm. $f_r^A = 0.30$  | 87F480 |
|  | <i>m</i> -Cresol   | air                      |                 | 0.42              |                |                            | CP/Ac-A.18  | $A = S$ ; $\lambda_{exc} = 546$ nm. $f_r^A = 0.30$  | 87F480 |
| <b>1.140 Dicyanobis(1,10-phenanthroline)ruthenium(II)</b>                                |  |                          |                 |                   |                |                            |             |   |        |
|  | MeOH   | O <sub>2</sub>           |                 | 0.68 <sup>T</sup> |                |                            | CL/Oc-14    | $A = TME$ ; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.141 (4,7-Diphenyl-1,10-phenanthroline)bis(1,10-phenanthroline)osmium(II) ion</b>    |  |                          |                 |                   |                |                            |             |   |        |
|  | MeOH   | O <sub>2</sub>           |                 | 0.78 <sup>T</sup> |                |                            | CL/Oc-14    | $A = TME$ ; $\lambda_{exc} = 488$ nm.   | 777221 |
| <b>1.142 Ergosterol</b>  |  |                          |                 |                   |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                              | 5.5 × 10 <sup>-4</sup>   |                 | 0.96*             |                |                            | PL/LI-60    | $S' = Np$ ; TD = p-MAP; rel. to $f_{\Delta}^T(S') = 0.55$ ; $\lambda_{exc} = 355$ nm.   | 87E055 |
|  |  |                          |                 | 0.85              |                |                            |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                              | 8.7 × 10 <sup>-4</sup>   |                 | 1.0*              |                |                            | PL/LI-60    | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm. Measured $P_T^{O_2}$ .  | 89A235 |
|  |  |                          |                 | 0.83              |                |                            |             |   |        |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment  | Ref.   |
|-------|---|-------------------|----------------|-----------------------------|-----------------------------|----------------------|-------------|--|--------|
| 1.143 | 9,10-Ethenoanthracene, 9-acethoxy-11,12-dibenzoyl-9,10-dihydro-       |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.62 <sup>T</sup>           | 0.9                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.7 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.144 | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-9,10-dimethoxy-   |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.17 <sup>T</sup>           | 0.9                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.2 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.145 | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-9-hydroxy-        |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.66 <sup>T</sup>           | 0.9                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.7 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.146 | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-9-methoxy-        |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.57 <sup>T</sup>           | 0.9                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.6 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.147 | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9-ethyl-9,10-dihydro-          |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.57 <sup>T</sup>           | 0.9                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.6 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.148 | 9,10-Ethenoanthracene-9-carbonitrile, 11,12-dibenzoyl-9,10-dihydro-   |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.44 <sup>T</sup>           | 0.6                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.7 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.149 | 9,10-Ethenoanthracene-9-carboxaldehyde, 11,12-dibenzoyl-9,10-dihydro- |                   |                |                             |                             |                      |             |  |        |
|       | C <sub>6</sub> H <sub>6</sub>   | air <sup>a</sup>  |                | 0.41 <sup>T</sup>           | 0.7                         |                      | PL/Ad-49,42 | A = DPBF; AC = BP; meas. Φ <sub>T</sub> (S) = 0.6 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 4.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.0 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. | 85B073 |
| 1.150 | Fluoranthene  |                   |                |                             |                             |                      |             |  |        |
|       | n-C <sub>6</sub> H <sub>14</sub>                                      | air               |                | 0.5                         |                             |                      | PL/Ad-43    | S' = An; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 264 nm. P <sub>1</sub> <sup>O<sub>2</sub></sup> = 1.  | 82E258 |
| 1.151 | Fluorene  |                   |                |                             |                             |                      |             |  |        |
|       | c-C <sub>6</sub> H <sub>12</sub>                                      | air               |                | 1.0                         |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm.  | 87E234 |
|       | C <sub>6</sub> H <sub>6</sub>   | air               |                | 0.74*                       |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55; λ <sub>exc</sub> = 355 nm.   | 87E234 |
|       |   |                   |                | 0.66                        |                             |                      |             |  |        |
|       | CH <sub>3</sub> CN  | air               |                | 1.0                         |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm.  | 87E234 |
|       | D <sub>2</sub> O (mic)  | O <sub>2</sub>    |                | 1.0                         |                             |                      | PL/LI-60    | S' = Np; TD = BP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm. [SDS] = 0.2-0.5 mol L <sup>-1</sup> .   | 87E234 |
|       | MeOH  | O <sub>2</sub>    |                | 0.09                        |                             |                      | CP/Oc-14    | A = TME; λ <sub>exc</sub> = 283-373 nm.  | 70F735 |
|       | MeOH  | O <sub>2</sub>    |                | 0.10                        |                             |                      | CP/Oc-14    | A = 2,5-DMF; λ <sub>exc</sub> = 283-373 nm.  | 70F735 |
|       | diox  | air               |                | 1.0                         |                             |                      | PL/LI-60    | S' = Np; TD = p-MAP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.0; λ <sub>exc</sub> = 355 nm.  | 87E234 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                | [O <sub>2</sub> ] | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method         | Comment   | Ref.   |
|---|--|-------------------|-------------------|----------------|----------------|----------------------------|----------------|---|--------|
| <b>1.152 Fluorene, 9-(phenylsulfonyl)-</b>  |  |                   |                   |                |                |                            |                |   |        |
|   | tert-BuOH                              | O <sub>2</sub>    | 0.035             |                |                |                            | CP/Pa-14       | A = S; P = 9-Fluorenone; $\lambda_{exc} = 360$ nm.  | 70F735 |
| <b>1.153 9-Fluorenone</b>   |  |                   |                   |                |                |                            |                |   |        |
|   | C <sub>6</sub> H <sub>6</sub>          | O <sub>2</sub>    | 0.82 <sup>T</sup> | 0.88           |                |                            | PL/Hp-52,42    | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.93$ . Measured $\phi_{\Delta} = 0.82$ , $P_T^{O_2} = 1$ and $\phi_P$ .                                  | 88E449 |
|   | C <sub>6</sub> H <sub>6</sub>          | O <sub>2</sub>    | 0.83 <sup>T</sup> | 0.89           |                |                            | PL/LI-56,42    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.93$ . Measured $P_T^{O_2} = 1$ .  | 88E449 |
|   | C <sub>6</sub> H <sub>6</sub>          | air               | 0.7 <sup>T</sup>  | 0.8            |                |                            | PL/LI,St-55,42 | S' = Ac; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.93^C$ .   | 84E287 |
|   | CD <sub>3</sub> OD                     | air <sup>a</sup>  | 0.02              |                |                |                            | CP/LI-56       | S' = RB; rel. to $\phi_{\Delta}(S') = 0.76$ . $P_T^{O_2} = 1$ ; measured ratio of $I_A$ at $\lambda_{exc}(S) = 367$ and $\lambda_{exc}(S') = 547$ nm. | 91F023 |
|   | MeOH                                   | O <sub>2</sub>    | 0.07              |                |                |                            | CP/Oc-14       | A = 2,5-DMF; $\lambda_{exc} = 283-373$ nm.  | 70F735 |
|   | MeOH                                   | O <sub>2</sub>    | 0.03              |                |                |                            | CP/Oc-14       | A = TME; $\lambda_{exc} = 283-373$ nm.  | 70F735 |
| <b>1.154 Fluorescein dianion</b>  |  |                   |                   |                |                |                            |                |   |        |
|   | c-C <sub>6</sub> H <sub>12</sub> (mic) | air               | 0.15              |                |                |                            | CP/Ac-14       | A = DPBF. Reverse micelles [DAP] = 8 × 10 <sup>-2</sup> mol L <sup>-1</sup> ; $\phi_{\Delta}$ decreased with added H <sub>2</sub> O.                  | 80N092 |
|   | EtOH                                   | air               | 0.03              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |
|   | EtOH                                   | air <sup>a</sup>  | 0.13              |                |                |                            | CP/Ac-14       | A = DPBF; $\lambda_{exc} = 488$ nm. Assumed $f_r^A = 2$ .   | 76R193 |
|   | H <sub>2</sub> O pH = 7                | air               | 0.03              |                |                |                            | CP/Ac-44       | S' = Eos; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.  | 83E113 |
|   | H <sub>2</sub> O                       | air <sup>a</sup>  | 0.06              |                |                |                            | CP/Ac-43,42    | S' = MB <sup>+</sup> ; A = 2,5-DMF; rel. to $\phi_{\Delta}(S') = 0.52$ ; used $\phi_T(S) = 0.05$ . Assumed $P_T^{O_2} = 1$ .                          | 737339 |
| <b>1.155 Fluorescein, dibromo-, dianion</b>   |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.29              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |
|   | H <sub>2</sub> O pH = 7                | air               | 0.42              |                |                |                            | CP/Ac-44       | S' = Eos; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.  | 83E113 |
| <b>1.156 Fluorescein, 4',5'-dibromo-2',7'-dinitro-, dianion (Eosin B)</b>             |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.37              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |
|   | H <sub>2</sub> O pH = 7                | air               | 0.52              |                |                |                            | CP/Ac-44       | S' = Eos; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.  | 83E113 |
| <b>1.157 Fluorescein, 2',7'-dibromo-4'-(hydroxymercuri)-, dianion (Mercurochrome)</b> |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.14              | 1.0            |                |                            | PL/LI-56,42    | S' = RB; rel. to $\phi_{\Delta}(S') = 0.76$ ; meas. $\phi_T(S) = 0.14$ .  | 92E001 |
|   | MeOH                                   | O <sub>2</sub>    | ~0.1              |                |                |                            | CP/Oc-43       | S' = Eos; A = 2,5-DMF; rel. to $\phi_{\Delta}(S') = 0.4$ .  | 90F289 |
| <b>1.158 Fluorescein, 2',7'-dichloro-, dianion</b>                                    |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.04              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |
|   | H <sub>2</sub> O pH = 7                | air               | 0.07              |                |                |                            | CP/Ac-44       | S' = Eos; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.  | 83E113 |
|   | H <sub>2</sub> O (mic)                 | air               | 0.06              |                |                |                            | CP/Ac-44       | S' = RB; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76^b$ . [SDS] = 0.1 mol L <sup>-1</sup> .   | 86N209 |
|   | H <sub>2</sub> O (mic)                 | air               | 0.03              |                |                |                            | CP/Ac-44       | S' = RB; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76^b$ . [CTAB] = 0.1 mol L <sup>-1</sup> .  | 86N209 |
| <b>1.159 Fluorescein, 4',5'-dichloro-, dianion</b>                                    |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.04              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |
|   | H <sub>2</sub> O pH = 7                | air               | 0.07              |                |                |                            | CP/Ac-44       | S' = Eos; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.  | 83E113 |
| <b>1.160 Fluorescein, diiodo-, dianion</b>  |  |                   |                   |                |                |                            |                |   |        |
|   | EtOH                                   | air               | 0.33              |                |                |                            | CP/Ac-44       | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ .  | 83E113 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                            | [O <sub>2</sub> ]       | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.   |
|--|------------------------------------|-------------------------|----------------|-----------------------------|-----------------------------|----------------------|-------------|---|--------|
| <b>1.160 Fluorescein, diiodo-, dianion—Continued</b>                                       |                                    |                         |                |                             |                             |                      |             |   |        |
|  | H <sub>2</sub> O pH = 7            | air                     |                | 0.48                        |                             |                      | CP/Ac-44    | S' = Eos; rel. to Φ <sub>Δ</sub> (S') = 0.57. A = RNO and ADPA.   | 83E113 |
| <b>1.161 Fluorescein, 2',4',5',7'-tetrabromo-, dianion (Eosin Y)</b>                       |                                    |                         |                |                             |                             |                      |             |   |        |
|  | CH <sub>3</sub> CN                 | air                     |                | 0.57 <sup>T</sup>           |                             |                      | CP/Pa-14    | A = DPF; P = 2,5-Diphenylfuran endoperoxide. Method adapted to allow for chain reaction.  | 87F440 |
|  | CH <sub>3</sub> COCH <sub>3</sub>  | air <sup>a</sup>        |                | 0.12 <sup>T</sup>           |                             |                      | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8. Reference value in CCl <sub>4</sub> .   | 82Z317 |
|  | EtOH                               | air                     |                | 0.60 <sup>T</sup>           | 0.92                        |                      | PL/LI-56,42 | S' = RB; rel. to Φ <sub>Δ</sub> (S') = 0.76; meas. ϕ <sub>T</sub> (S) = 0.65.   | 92E001 |
|  | EtOH                               | 9.9 × 10 <sup>-3</sup>  |                | 0.42 <sup>T</sup>           | 0.64                        |                      | CP/Oc-43,42 | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50; used ϕ <sub>T</sub> (S) = 0.65 <sup>d</sup> . Used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 84F191 |
|  | D <sub>2</sub> O<br>pD = 8.2       | air                     |                | 0.58 <sup>T</sup>           |                             |                      | PL/LI-56    | rel. to Eos in EtOH, unclear what reference value was used  | 91N118 |
|  | D <sub>2</sub> O (mic)<br>pD = 8.2 | air                     |                | 0.24 <sup>T</sup>           |                             |                      | PL/LI-56    | rel. to Eos in EtOH, unclear what reference value was used; CPC micelles.   | 91N118 |
|  | H <sub>2</sub> O                   | air <sup>a</sup>        |                | 0.57 <sup>T</sup>           | 0.89                        |                      | CP/Ac-43,42 | S' = MB <sup>+</sup> ; A = 2,5-DMF; rel. to Φ <sub>Δ</sub> (S') = 0.52; used ϕ <sub>T</sub> (S) = 0.64. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.        | 737339 |
|  | H <sub>2</sub> O (mic)             | air                     |                | 0.54 <sup>T</sup>           |                             |                      | CP/Ac-44    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76 <sup>b</sup> . [SDS] = 0.1 mol L <sup>-1</sup> .  | 86N209 |
|  | H <sub>2</sub> O (mic)             | air                     |                | 0.14 <sup>T</sup>           |                             |                      | CP/Ac-44    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76 <sup>b</sup> . [CTAB] = 0.1 mol L <sup>-1</sup> .   | 86N209 |
|  | MeOH                               | air <sup>a</sup>        |                | 0.26 <sup>T</sup>           |                             |                      | CP/Ac-43    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76.  | 90F251 |
|  | MeOH                               | air <sup>a</sup>        |                | 0.30 <sup>T</sup>           |                             |                      | CP/Ac-43    | A = DPBF. Rel. to Φ <sub>Δ</sub> = 0.32 for eosin disodium salt in ethanol.   | 90F251 |
|  | MeOH                               | 1.06 × 10 <sup>-2</sup> |                | 0.42 <sup>T</sup>           | 0.64                        |                      | CP/Oc-43,39 | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50; used ϕ <sub>T</sub> (S) = 0.66 <sup>f</sup> . Used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 84F191 |
| <b>1.162 Fluorescein, 2',4',5',7'-tetrabromo-, benzyl ester, monoanion</b>                 |                                    |                         |                |                             |                             |                      |             |   |        |
|  | MeOH                               | air <sup>a</sup>        |                | 0.36                        |                             |                      | CP/Ac-43    | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32. Rel. to S' in ethanol.  | 90F251 |
|  | MeOH                               | air <sup>a</sup>        |                | 0.32                        |                             |                      | CP/Ac-43    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76.  | 90F251 |
| <b>1.163 Fluorescein, 2',4',5',7'-tetrabromo-, p-isopropylbenzyl ester, monoanion</b>      |                                    |                         |                |                             |                             |                      |             |   |        |
|  | MeOH                               | air <sup>a</sup>        |                | 0.32                        |                             |                      | CP/Ac-43    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76.  | 90F251 |
|  | MeOH                               | air <sup>a</sup>        |                | 0.36                        |                             |                      | CP/Ac-43    | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32. Rel. to S' in ethanol.  | 90F251 |
| <b>1.164 Fluorescein, 2',4',5',7'-tetrabromo-, methyl ester, protonated</b>                |                                    |                         |                |                             |                             |                      |             |   |        |
|  | diox                               | air <sup>a</sup>        |                | 0.26                        |                             |                      | CP/Ac-43    | S' = O-Methyl Rose Bengal methyl ester; A = TPCP; rel. to Φ <sub>Δ</sub> (S') = 0.70. Soln. contg. 10 <sup>-3</sup> mol L <sup>-1</sup> HCl.                        | 90F251 |
|  | diox                               | air <sup>a</sup>        |                | 0.30                        |                             |                      | CP/Ac-43    | S' = Eos; A = TPCP; rel. to Φ <sub>Δ</sub> (S') = 0.32. Soln. contg. 10 <sup>-3</sup> mol L <sup>-1</sup> HCl. rel. to S' in ethanol.                               | 90F251 |
| <b>1.165 Fluorescein, 2',4',5',7'-tetrabromo-, methyl ester, monoanion</b>                 |                                    |                         |                |                             |                             |                      |             |   |        |
|  | MeOH                               | air <sup>a</sup>        |                | 0.32                        |                             |                      | CP/Ac-43    | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32. Rel. to S' in ethanol.  | 90F251 |
|  | MeOH                               | air <sup>a</sup>        |                | 0.28                        |                             |                      | CP/Ac-43    | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76.  | 90F251 |
| <b>1.166 Fluorescein, 2',4',5',7'-tetrabromo-3,4,5,6-tetrachloro-, dianion (Phloxin B)</b> |                                    |                         |                |                             |                             |                      |             |   |        |
|  | EtOH                               | air                     |                | 0.40                        |                             |                      | CP/Ac-44    | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32.   | 83E113 |
|  | H <sub>2</sub> O pH = 7            | air                     |                | 0.65                        |                             |                      | CP/Ac-44    | S' = Eos; rel. to Φ <sub>Δ</sub> (S') = 0.57. A = RNO and ADPA.   | 83E113 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]     | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method       | Comment  | Ref.   |
|---|--|-----------------------|----------------|-----------------------------|-----------------------------|----------------------|--------------|--|--------|
| <b>1.166 Fluorescein, 2',4',5',7'-tetrabromo-3,4,5,6-tetrachloro-, dianion (Phloxin B)—Continued</b>    |  |                       |                |                             |                             |                      |              |  |        |
|   | H <sub>2</sub> O (mic)                                     | air                   |                | 0.35                        |                             |                      | CP/Ac-44     | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76 <sup>b</sup> . [CTAB] = 0.1 mol L <sup>-1</sup> .  | 86N209 |
|   | H <sub>2</sub> O (mic)                                     | air                   |                | 0.39                        |                             |                      | CP/Ac-44     | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76 <sup>b</sup> . [SDS] = 0.1 mol L <sup>-1</sup> .   | 86N209 |
| <b>1.167 Fluorescein, 2',4',5',7'-tetrachloro-, dianion</b>   |  |                       |                |                             |                             |                      |              |  |        |
|   | EtOH   | air                   |                | 0.05                        |                             |                      | CP/Ac-44     | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32.  | 83E113 |
|   | H <sub>2</sub> O pH = 7                                    | air                   |                | 0.05                        |                             |                      | CP/Ac-44     | S' = Eos; rel. to Φ <sub>Δ</sub> (S') = 0.57. A = RNO and ADPA.  | 83E113 |
| <b>1.168 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo- (Rose Bengal lactone)</b>              |  |                       |                |                             |                             |                      |              |  |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> /MeOH (99:1) | air                   |                | 0.65 <sup>T</sup>           |                             |                      | CP/Ac-14     | A = DPBF; λ <sub>exc</sub> = 546 nm. [O <sub>2</sub> ] varied.   | 87F479 |
|   | CCl <sub>4</sub> /MeOH (97:3)                              | air                   |                | 0.71 <sup>T</sup>           |                             |                      | CP/Ac-14     | A = DPBF; λ <sub>exc</sub> = 546 nm. [O <sub>2</sub> ] varied.   | 87F479 |
|   | DMF  | air                   |                | 0.4 <sup>T</sup>            |                             |                      | CP/Ac-14,A18 | A = DPBF.  | 79F412 |
| <b>1.169 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, dianion (Rose Bengal dianion, RB)</b> |  |                       |                |                             |                             |                      |              |  |        |
|   | tert-BuOH  | O <sub>2</sub>        |                | 0.80 <sup>T</sup>           |                             |                      | CP/Pa-14     | A = 9-(Phenylsulfonyl)fluorene anion; P = 9-Fluorenone; λ <sub>exc</sub> = 546 nm.   | 707250 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH           | air                   |                | 0.95 <sup>T</sup>           |                             |                      | CP/Ac-14     | A = DPBF; λ <sub>exc</sub> = 546 nm. [O <sub>2</sub> ] varied.   | 87F479 |
|   | CH <sub>3</sub> CN   | air                   |                | 0.54 <sup>T</sup>           |                             |                      | CP/Ac-14     | A = DPBF.  | 90E215 |
|   | CH <sub>3</sub> CN   | air <sup>a</sup>      |                | 0.83 <sup>T</sup>           |                             |                      | CP/Pa-14     | A = DPF; P = 2,5-Diphenylfuran endoperoxide. Method adapted to allow for chain reaction.   | 87F440 |
|   | EtOH   | air <sup>a</sup>      |                | 0.68 <sup>T</sup>           | 0.8                         |                      | CP/Pa-43,42  | A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 555 nm; used φ <sub>T</sub> (S) = 0.90 <sup>d</sup> . Rel. to RB in methanol.                                  | 86F462 |
|   | EtOH   | air                   |                | 0.86 <sup>T</sup>           | 1                           |                      | CP/Ac-44,42  | S' = Eos; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.32; used φ <sub>T</sub> (S) = 0.90 <sup>d</sup> .  | 83E113 |
|   | D <sub>2</sub> O pH = 7.4                                  | air                   |                | 0.62 <sup>T</sup>           |                             |                      | PL/LI-56     | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.62. independent of λ = 308 and 532 nm.  | 91R177 |
|   | D <sub>2</sub> O pD = 8.2                                  | air                   |                | 0.75 <sup>T</sup>           |                             |                      | PL/LI-56     | rel. to Φ <sub>Δ</sub> (S') = 0.75. rel. to RB in EtOH, cor. for solvent k <sub>r</sub> .  | 91N118 |
|   | D <sub>2</sub> O (mic) pD = 8.2                            | air                   |                | 0.75 <sup>T</sup>           |                             |                      | PL/LI-56     | rel. to Φ <sub>Δ</sub> (S') = 0.75. rel. to RB in EtOH, cor. for solvent k <sub>r</sub> ; CPC micelles.  | 91N118 |
|   | H <sub>2</sub> O   | air or O <sub>2</sub> |                | 0.76                        |                             |                      |              | See Table 4.   |        |
|   | H <sub>2</sub> O pH = 7                                    | air                   |                | 0.75 <sup>T</sup>           |                             |                      | CP/Ac-44     | S' = Eos; rel. to Φ <sub>Δ</sub> (S') = 0.57. A = RNO and ADPA.  | 83E113 |
|   | H <sub>2</sub> O pH = 7.0                                  | O <sub>2</sub>        |                |                             | 0.76                        |                      | PL/Ad,St-48  | A = ADPA; λ <sub>exc</sub> = 532 nm. used Δε <sub>T</sub> (S) = 4900 L mol <sup>-1</sup> cm <sup>-1</sup> at 600 nm; assumed P <sub>S<sup>0</sup></sub> <sup>2</sup> = 0 and measured P <sub>T<sup>0</sup></sub> <sup>2</sup> = 1. | 87A043 |
|   | H <sub>2</sub> O pH = 7.4                                  | O <sub>2</sub>        |                | 0.75 <sup>T</sup>           |                             |                      | CP/Ac-14     | A = TrpH; λ <sub>exc</sub> = 540 nm. 1.6% NaCl in phosphate buffer.  | 88N170 |
|   | H <sub>2</sub> O pH = 7.4                                  | O <sub>2</sub>        |                | 0.74 <sup>T</sup>           |                             |                      | CP/Oc-14     | A = Im; λ <sub>exc</sub> = 540 nm. 1.6% NaCl in phosphate buffer.  | 88N170 |
|   | i-octane/H <sub>2</sub> O (96:4) (mic)                     | O <sub>2</sub>        |                | 0.81 <sup>T</sup>           | 1                           |                      | PL/Hp-53,42  | meas. φ <sub>T</sub> (S) = 0.78; λ <sub>exc</sub> = 355 nm. Soln. cont. 0.1 mol L <sup>-1</sup> AOT; meas. φ <sub>F</sub> = 0.057.   | 91N191 |
|   | i-octane/H <sub>2</sub> O (96:4) (mic)                     | O <sub>2</sub>        |                | 0.80 <sup>T</sup>           | 1                           |                      | PL/Hp-52,42  | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.80; meas. φ <sub>T</sub> (S) = 0.78; λ <sub>exc</sub> = 355 nm. Soln. cont. 0.1 mol L <sup>-1</sup> AOT.  | 91N191 |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]     | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.             |
|---|--|-----------------------|-------------------|----------------|----------------|----------------------------|-------------|---|------------------|
| <b>1.169 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, dianion (Rose Bengal dianion, RB)—Continued</b>   |  |                       |                   |                |                |                            |             |   |                  |
|   | H <sub>2</sub> O/MeOH<br>(1:1) pH = 7                            | O <sub>2</sub>        | 0.75 <sup>T</sup> |                |                |                            | CP/Pa-14    | A = TrpH; $\lambda_{exc}$ = 555 nm.   | 87F104           |
|   | MeOH   | air or O <sub>2</sub> | 0.80              |                |                |                            |             | See Table 4.  |                  |
|   | MeOH   | air                   | 0.81 <sup>T</sup> |                |                |                            | CP/Ac-14    | A = DPBF.   | 90E215           |
|   | MeOH   | air                   | 0.77 <sup>T</sup> |                |                |                            | CP/Ac-14    | A = DPBF.   | 90F157           |
|   | MeOH   | air <sup>a</sup>      | 0.82 <sup>T</sup> |                |                |                            | CP/Ac-43    | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S')$ = 0.32.<br>Rel. to S' in ethanol; $\phi_{\Delta}$ = 0.93 for 'pure' RB<br>rel. to Eos; $\phi_{\Delta}$ = 0.87 for 'commercial' RB rel.<br>to Eos; $\phi_{\Delta}$ = 0.81 for 'pure' RB rel. to $\phi_{\Delta}$ =<br>0.76 for commercial RB. | 90F251           |
|   | MeOH   | $1.06 \times 10^{-2}$ | 0.79 <sup>T</sup> | ~1             |                |                            | CP/Oc-43,39 | S' = MB <sup>+</sup> ; A = TME; rel. to $\phi_{\Delta}(S')$ = 0.50;<br>used $\phi_T(S)$ = 0.80 <sup>T</sup> . Used $P_T^{O_2}$ = 1.   | 84F191           |
|   | MeOH   | O <sub>2</sub>        | 0.80 <sup>T</sup> |                |                |                            | CL/Oc-14    | A = TME; $\lambda_{exc}$ = 488 nm.  | 777221           |
|   | MeOH   | O <sub>2</sub>        | 0.80 <sup>T</sup> |                |                |                            | CP/Oc-14    | A = TME; $\lambda_{exc}$ = 283-373 nm.  | 70F735           |
|   | MeOH   | O <sub>2</sub>        | 0.82 <sup>T</sup> |                |                |                            | CP/Oc-14    | A = 2,5-DMF; $\lambda_{exc}$ = 283-373 nm.  | 70F735           |
|   | MeOH/<br>C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub><br>(97:3) | air                   | 0.91 <sup>T</sup> |                |                |                            | CP/Ac-14    | A = DPBF. [O <sub>2</sub> ] varied.   | 87F479           |
|   | 2-PrOH   | air                   | 0.76 <sup>T</sup> |                |                |                            | CP/Ac-14    | A = DPBF.   | 90E215           |
| <b>1.170 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, 6-O-acetyl-, ethyl ester</b>                      |  |                       |                   |                |                |                            |             |   |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>                                  | O <sub>2</sub>        | 0.61              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 561 nm.   | 84F297<br>85F152 |
| <b>1.171 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester</b>                                  |  |                       |                   |                |                |                            |             |   |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub> /<br>MeOH (8:2)                  | O <sub>2</sub>        | 0.37              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 566 nm.   | 85F171           |
| <b>1.172 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, monoanion</b>                       |  |                       |                   |                |                |                            |             |   |                  |
|   | MeOH   | air <sup>a</sup>      | 0.94              |                |                |                            | CP/Ac-43    | S' = Eos; A = DPBF; rel. to $\phi_{\Delta}(S')$ = 0.32.<br>Rel. to S' in ethanol.   | 90F251           |
|   | MeOH   | air <sup>a</sup>      | 0.82              |                |                |                            | CP/Ac-43    | S' = RB; A = DPBF; rel. to $\phi_{\Delta}(S')$ = 0.76.  | 90F251           |
|   | MeOH   | O <sub>2</sub>        | 0.72              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 566 nm.   | 85F171           |
| <b>1.173 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, benzyltriphenylphosphonium salt</b> |  |                       |                   |                |                |                            |             |   |                  |
|   | MeOH   | O <sub>2</sub>        | 0.76              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 561 nm.   | 88F161           |
| <b>1.174 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, diphenyliodonium salt</b>           |  |                       |                   |                |                |                            |             |   |                  |
|   | MeOH   | O <sub>2</sub>        | 0.74              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 561 nm.   | 88F161           |
| <b>1.175 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, diphenylmethylsulfonium salt</b>    |  |                       |                   |                |                |                            |             |   |                  |
|   | MeOH   | O <sub>2</sub>        | 0.73              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 561 nm.   | 88F161           |
| <b>1.176 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, triethylammonium salt</b>           |  |                       |                   |                |                |                            |             |   |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>                                  | O <sub>2</sub>        | 0.67              |                |                |                            | CP/Pa-43    | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P =<br>1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S')$ =<br>0.76; $\lambda_{exc}$ = 561 nm.   | 84F297<br>85F152 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                           | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method   | Comment  | Ref.             |
|---|-----------------------------------|-------------------|----------------|-----------------------------|-----------------------------|----------------------|----------|--|------------------|
| <b>1.176 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, triethylammonium salt—Continued</b> |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | MeOH                              | O <sub>2</sub>    | 0.74           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
| <b>1.177 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, 2,4,6-triphenylpyrylium salt</b>    |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | MeOH                              | O <sub>2</sub>    | 0.70           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 88F161           |
| <b>1.178 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(benzyltriphenylphosphonium) salt</b>          |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | MeOH                              | O <sub>2</sub>    | 0.74           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 88F161           |
| <b>1.179 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(diphenyliodonium) salt</b>                    |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | MeOH                              | O <sub>2</sub>    | 0.66           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 88F161           |
| <b>1.180 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(triethylammonium) salt</b>                    |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>   | O <sub>2</sub>    | 0.48           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
|   | MeOH                              | O <sub>2</sub>    | 0.72           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
| <b>1.181 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, complexed with dicyclohexyl-18-crown-8</b>        |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>   | air <sup>a</sup>  | 0.76           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 559 nm. Rel. to S' in methanol. | 86F462           |
|   | CH <sub>3</sub> COCH <sub>3</sub> | air <sup>a</sup>  | 0.70           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 557 nm. Rel. to S' in methanol. | 86F462           |
|   | CHCl <sub>3</sub>                 | air <sup>a</sup>  | 0.76           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 559 nm. Rel. to S' in methanol. | 86F462           |
|   | CHCl <sub>3</sub>                 | air <sup>a</sup>  | 0.36           |                             |                             |                      | CP/Ac-14 | A = DPBF; λ <sub>exc</sub> = 560 nm.   | 79F104           |
|   | MeOH                              | air <sup>a</sup>  | 0.63           |                             |                             |                      | CP/Ac-14 | A = DPBF; λ <sub>exc</sub> = 560 nm.   | 79F104           |
| <b>1.182 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, ethyl ester</b>                                   |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>   | O <sub>2</sub>    | 0.61           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
|   | MeOH                              | O <sub>2</sub>    | 0.73           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
| <b>1.183 Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, ethyl ester, triethylammonium salt</b>            |                                   |                   |                |                             |                             |                      |          |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>   | O <sub>2</sub>    | 0.71           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |
|   | MeOH                              | O <sub>2</sub>    | 0.74           |                             |                             |                      | CP/Pa-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 561 nm.                         | 84F297<br>85F152 |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]                             | $\phi_{\Delta}$  | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.             |
|-------|--|---|------------------|-------------------|----------------|----------------------------|-------------|---|------------------|
| 1.184 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, <i>p</i> -isopropylbenzyl ester, protonated | diox  | air <sup>a</sup> | 0.80              |                |                            | CP/Ac-43    | $S' = Eos; A = TPCP$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Soln. contg. $10^{-3}$ mol L <sup>-1</sup> HCl; rel. to S' in ethanol.  | 90F251           |
| 1.185 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, <i>p</i> -isopropylbenzyl ester, monoanion  | MeOH  | air <sup>a</sup> | 0.90              |                |                            | CP/Ac-43    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Rel. to S' in ethanol.  | 90F251           |
|       |  | MeOH  | air <sup>a</sup> | 0.79              |                |                            | CP/Ac-43    | $S' = RB; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 90F251           |
| 1.186 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, <i>O</i> -methyl-, methyl ester             | diox  | air <sup>a</sup> | 0.80              |                |                            | CP/Ac-43    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Rel. to S' in ethanol.  | 90F251           |
|       |  | MeOH  | air <sup>a</sup> | 0.70              |                |                            | CP/Ac-43    | $S' = RB; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 90F251           |
|       |  | MeOH  | air <sup>a</sup> | 0.80              |                |                            | CP/Ac-43    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Rel. to S' in ethanol.  | 90F251           |
| 1.187 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, methyl ester, protonated                    | diox  | air <sup>a</sup> | 0.75              |                |                            | CP/Ac-43    | $S' = O$ -Methyl Rose Bengal methyl ester; A = TPCP; rel. to $\phi_{\Delta}(S') = 0.70$ . Soln. contg. $10^{-3}$ mol L <sup>-1</sup> HCl; rel. to S' in methanol.   | 90F251           |
|       |  | diox  | air <sup>a</sup> | 0.86              |                |                            | CP/Ac-43    | $S' = Eos; A = TPCP$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Soln. contg. $10^{-3}$ mol L <sup>-1</sup> HCl; rel. to S' in ethanol.  | 90F251           |
| 1.188 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, methyl ester, monoanion                     | MeOH  | air <sup>a</sup> | 0.80              |                |                            | CP/Ac-43    | $S' = RB; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 90F251           |
|       |  | MeOH  | air <sup>a</sup> | 0.91              |                |                            | CP/Ac-43    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ . Rel. to S' in ethanol.  | 90F251           |
| 1.189 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, octyl ester, tributylammonium salt          | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | O <sub>2</sub>   | 0.40              |                |                            | CP/Pa-43    | $S' = RB; A = 2,3$ -Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 561$ nm.   | 84F297<br>85F152 |
| 1.190 | Fluorescein, 2',4',5',7'-tetraiodo-, dianion (Erythrosin)  | CH <sub>3</sub> CN                            | air              | 0.68 <sup>T</sup> |                |                            | CP/Pa-14    | A = DPF; P = 2,5-Diphenylfuran endoperoxide. Method adapted to allow for chain reaction.  | 87F440           |
|       |  | DMF   | air <sup>a</sup> | 0.54 <sup>T</sup> |                |                            | CP/Ac-43    | $S' = RB; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 88F618           |
|       |  | EtOH  | air              | 0.69 <sup>T</sup> |                |                            | CP/Ac-44    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ .   | 83E113           |
|       |  | H <sub>2</sub> O pH = 7                       | air              | 0.63 <sup>T</sup> |                |                            | CP/Ac-44    | $S' = Eos$ ; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.   | 83E113           |
|       |  | H <sub>2</sub> O                              | air <sup>a</sup> | 0.68 <sup>T</sup> | 0.68           |                            | CP/Ac-43,42 | $S' = MB^+$ ; A = 2,5-DMF; rel. to $\phi_{\Delta}(S') = 0.52$ ; used $\phi_T(S) = 1.0$ . Assumed $P_T^{O_2} = 1$ .  | 737339           |
|       |  | MeOD  | $\sim 10^{-3}$   | 0.60 <sup>T</sup> | 0.57           |                            | PL/LI-56,42 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.53$ ; meas. $\phi_T(S) = 1.1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ ; rel. to S' in EtOH. Recalcd. value = 0.70 using $\phi_{\Delta}(S') = 0.64$ [88Z155]. | 88A165           |
| 1.191 | Fluorescein, tribromo-, dianion  | EtOH  | air              | 0.32              |                |                            | CP/Ac-44    | $S' = Eos; A = DPBF$ ; rel. to $\phi_{\Delta}(S') = 0.32$ .   | 83E113           |
|       |  | H <sub>2</sub> O pH = 7                       | air              | 0.44              |                |                            | CP/Ac-44    | $S' = Eos$ ; rel. to $\phi_{\Delta}(S') = 0.57$ . A = RNO and ADPA.   | 83E113           |
| 1.192 | Furan, 2,5-di(2-thienyl)-  | EtOH  | O <sub>2</sub>   | $\sim 0.1$        | $\sim 1$       |                            | PL/Ac-14,42 | A = DPBF; meas. $\phi_T(S) = 0.10^f$ ; $\lambda_{exc} = 353$ nm. $P_T^{O_2} = 1$ , $p_A = 0.75$ .   | 85N020           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]     | $\phi_{\Delta}$    | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.             |
|-------|---|-----------------------|--------------------|-------------------|----------------|----------------------------|-------------|--|------------------|
| 1.193 | Furo[2,3- <i>f</i> ][1]benzopyran-7-one, 8-acetyl- (3-Acetoallopssoralen)                     |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.63*              | 0.55 <sup>T</sup> | 0.81           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.68$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121           |
| 1.194 | Furo[2,3- <i>f</i> ][1]benzopyran-7-one, 4,9-dimethyl- (4,7-Dimethylallopssoralen, 4,7-DMAPs) |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | $1.91 \times 10^{-3}$ | 0.073*             | 0.064             | 0.49           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.13$ ; $\lambda_{exc} = 355$ nm.  | 87E497           |
| 1.195 | Furo[2,3- <i>f</i> ][1]benzopyran-7-one, 2,4,9-trimethyl- (4,7,5'-Trimethylallopssoralen)     |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | $1.91 \times 10^{-3}$ | 0.14*              | 0.12              | 0.68           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.18$ ; $\lambda_{exc} = 355$ nm.  | 87E497           |
|       | H <sub>2</sub> O<br>pH = 7.3  | $2.65 \times 10^{-4}$ |                    |                   |                |                            | CP/Pa-43    | $S' = 4,7$ -DMAPs; A = Im; P = Imidazole endoperoxide; meas. $\phi_A(S)/\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 365$ nm. RNO as monitor of P.   | 87E497           |
| 1.196 | Furo[2,3- <i>f</i> ][1]benzopyran-7-one, 3,4,9-trimethyl- (4,7,4'-Trimethylallopssoralen)     |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | $1.91 \times 10^{-3}$ | 0.083*             | 0.073             | 0.26           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.28$ ; $\lambda_{exc} = 355$ nm.  | 87E497           |
|       | H <sub>2</sub> O<br>pH = 7.3  | $2.65 \times 10^{-4}$ |                    |                   |                |                            | CP/Pa-43    | $S' = 4,7$ -DMAPs; A = Im; P = Imidazole endoperoxide; meas. $\phi_A(S)/\phi_{\Delta}(S') = 0.38$ ; $\lambda_{exc} = 365$ nm. RNO as monitor of P.   | 87E497           |
| 1.197 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 3-acetyl- (3-Acetoangelicin)                         |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.46*              | 0.40 <sup>T</sup> | 0.73           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.54$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121           |
| 1.198 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 4,6-dimethyl- (6,4-Dimethylangelicin)                |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.01 <sup>T</sup>  | 0.25              |                |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.04$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121           |
| 1.199 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 4,8-dimethyl- (4,5'-Dimethylangelicin)               |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.02 <sup>T</sup>  | 0.25              |                |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.08$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121           |
|       | H <sub>2</sub> O<br>pH = 7.3  | air <sup>a</sup>      | 0.02 <sup>T</sup>  |                   |                |                            | CP/Pa-43    | $S' = Ang$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.02^b$ ; $\lambda_{exc} = 365$ nm. Measured $\phi_T = 0.063$ in MeOH; RNO as monitor of P.                  | 84E794           |
| 1.200 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 4,9-dimethyl- (4,4'-Dimethylangelicin)               |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.02 <sup>T</sup>  | 0.18              |                |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.11$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121           |
|       | H <sub>2</sub> O<br>pH = 7.3  | O <sub>2</sub>        | 0.03 <sup>T</sup>  |                   |                |                            | CP/Pa-43    | $S' = Ang$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.02^b$ ; $\lambda_{exc} = 365$ nm. Measured $\phi_T = 0.11$ in EtOH; RNO as monitor of P; $P_T^{O_2} = 1$ . | 84F111<br>84E794 |
| 1.201 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 5,9-dimethyl- (4',5-Dimethylangelicin)               |                       |                    |                   |                |                            |             |  |                  |
|       | H <sub>2</sub> O<br>pH = 7.3  | O <sub>2</sub>        | 0.007 <sup>T</sup> |                   |                |                            | CP/Pa-43    | $S' = Ang$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.02^b$ ; $\lambda_{exc} = 365$ nm. Measured $\phi_T = 0.12$ in EtOH; RNO as monitor of P; $P_T^{O_2} = 1$ . | 84F111<br>84E794 |
| 1.202 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 6,9-dimethyl- (6,4'-Dimethylangelicin)               |                       |                    |                   |                |                            |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>        | 0.01 <sup>T</sup>  | 0.14              |                |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.07$ ; $\lambda_{exc} = 355$ nm.  | 88E121           |
| 1.203 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 4-methyl- (4-Methylangelicin)                        |                       |                    |                   |                |                            |             |  |                  |
|       | H <sub>2</sub> O<br>pH = 7.3  | air <sup>a</sup>      | 0.02 <sup>T</sup>  |                   |                |                            | CP/Pa-43    | $S' = Ang$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.02^b$ ; $\lambda_{exc} = 365$ nm. Measured $\phi_T = 0.05$ in MeOH; RNO as monitor of P                    | 84E794           |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]                | Φ <sub>Δ</sub>   | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment  | Ref.             |
|-------|--|----------------------------------|------------------|-----------------------------|-----------------------------|----------------------|-------------|--|------------------|
| 1.204 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 5-methyl- (5-Methylangelicin)   | H <sub>2</sub> O<br>pH = 7.3     | air <sup>a</sup> | 0.02 <sup>T</sup>           |                             |                      | CP/Pa-43    | S' = Ang; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.02 <sup>b</sup> ; λ <sub>exc</sub> = 365 nm. Measured Φ <sub>T</sub> = 0.12 in MeOH; RNO as monitor of P   | 84E794           |
| 1.205 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 8-methyl- (8'-Methylangelicin)  | H <sub>2</sub> O<br>pH = 7.3     | air <sup>a</sup> | 0.007 <sup>T</sup>          |                             |                      | CP/Pa-43    | S' = Ang; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.02 <sup>b</sup> ; λ <sub>exc</sub> = 365 nm. Measured Φ <sub>T</sub> = 0.08 in EtOH; RNO as monitor of P   | 84E794           |
| 1.206 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 9-methyl- (4'-Methylangelicin)  | H <sub>2</sub> O<br>pH = 7.3     | O <sub>2</sub>   | 0.01 <sup>T</sup>           |                             |                      | CP/Pa-43    | S' = Ang; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.02 <sup>b</sup> ; λ <sub>exc</sub> = 365 nm. Measured Φ <sub>T</sub> = 0.08 in EtOH; RNO as monitor of P; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 84F111<br>84E794 |
| 1.207 | Furo[2,3- <i>h</i> ][1]benzopyran-2-one, 4,6,9-trimethyl- (6,4,4'-Trimethylangelicin)  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.02 <sup>T</sup>           | 0.16                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.13; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.208 | Furo[3,2- <i>f</i> ][1]benzopyran-7-one (Isopseudopsoralen)  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.11*<br>0.10 <sup>T</sup>  | 0.67                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.15; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.209 | Furo[3,2- <i>f</i> ][1]benzopyran-7-one, 8-acetyl- (3-Acetoisopseudopsoralen)  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.73*<br>0.64 <sup>T</sup>  | 0.99                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.65; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.210 | Furo[3,2- <i>g</i> ][1]benzopyran-7-one, 2-acetyl-5,9-dimethyl- (5'-Aceto-4,8-dimethylpsoralen)                                    | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.43*<br>0.38 <sup>T</sup>  | 0.72                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.52; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.211 | Furo[3,2- <i>g</i> ][1]benzopyran-7-one, 2-acetyl-9-methyl- (5'-Aceto-8-methylpsoralen)  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.13*<br>0.11 <sup>T</sup>  | 0.39                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.28; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.212 | Furo[3,2- <i>h</i> ][1]benzopyran-8-one, 7-acetyl- (3-Acetopseudoisopsoralen)  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>   | 0.63*<br>0.55 <sup>T</sup>  | 0.99                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.56; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.213 | Helianthrene   |                                  |                  |                             |                             |                      |             |  |                  |
|       | n-C <sub>5</sub> H <sub>12</sub>   | air                              |                  | 0.52                        |                             |                      | CP/Ac-A.18  | A = S; λ <sub>exc</sub> = 546 nm.  | 87F480           |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air                              |                  | 0.56                        |                             |                      | CP/Ac-14,38 | A = S; meas. Φ <sub>T</sub> (S) = 0.46; λ <sub>exc</sub> = 546 nm. f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, [O <sub>2</sub> ] varied, (f <sub>Δ</sub> <sup>S</sup> + f <sub>Δ</sub> <sup>T</sup> )f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.0.   | 87F479           |
|       | CCl <sub>4</sub>   | air                              |                  | 0.50                        |                             |                      | CP/Ac-14    | A = S; λ <sub>exc</sub> = 546 nm. [O <sub>2</sub> ] varied, f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 87F479           |
|       | CH <sub>3</sub> COCH <sub>3</sub>  | air                              |                  | 0.50                        |                             |                      | CP/Ac-A.18  | A = S; λ <sub>exc</sub> = 546 nm.  | 87F480           |
|       | MeOH /C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub><br>(97:3)  | air                              |                  | 0.42                        |                             |                      | CP/Ac-A.18  | A = S; λ <sub>exc</sub> = 546 nm.  | 87F480           |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH   | air                              |                  | 0.24                        |                             |                      | CP/Ac-A.18  | A = S; λ <sub>exc</sub> = 546 nm.  | 87F480           |
|       | m-Cresol   | air                              |                  | 0.18                        |                             |                      | CP/Ac-A.18  | A = S; λ <sub>exc</sub> = 546 nm.  | 87F480           |
| 1.214 | ( <i>E,E,E</i> )-2,4,6-Heptatrienal, 5-methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)- ( <i>all-trans</i> -C <sub>17</sub> aldehyde) | c-C <sub>6</sub> H <sub>12</sub> | air              | 0.66 <sup>T</sup>           | 1.0                         |                      | PL/Ad-49,39 | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 5 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 3.4 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , Φ <sub>T</sub> (S) = 0.66 <sup>c</sup> , ε <sub>T</sub> (AC) = 63000 L mol <sup>-1</sup> cm <sup>-1</sup> at 410 nm. | 85F041           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ]         | ϕ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.   |
|--|---|---------------------------|-------------------|-----------------------------|-----------------------------|----------------------|-------------|---|--------|
| <b>1.214 (E,E,E)-2,4,6-Heptatrienal, 5-methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)- (all-trans-C<sub>17</sub> aldehyde)—Continued</b> |   |                           |                   |                             |                             |                      |             |   |        |
|  | c-C <sub>6</sub> H <sub>12</sub>              | O <sub>2</sub>            | 0.72 <sup>T</sup> | 1                           |                             |                      | PL/Ad 49,42 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 5.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 3.4 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ϕ <sub>T</sub> (S) = 0.66 <sup>f</sup> , ϕ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.   | 84F005 |
|  | MeOH  | air                       | -0.4 <sup>T</sup> | 1                           |                             |                      | PL/Ad-49,39 | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 1 × 10 <sup>5</sup> s <sup>-1</sup> , k <sub>A</sub> = 8 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ϕ <sub>T</sub> (S) = 0.41 <sup>c</sup> , ε <sub>T</sub> (AC) = 57000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm.  | 85F041 |
|  | MeOH  | O <sub>2</sub>            | 0.42 <sup>T</sup> | 1.0                         |                             |                      | PL/Ad-49,42 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 1.0 × 10 <sup>5</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.1 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ϕ <sub>T</sub> (S) = 0.41 <sup>f</sup> , ϕ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.   | 84F005 |
| <b>1.215 Heterocoerdianthrone (HCD)</b>  |   |                           |                   |                             |                             |                      |             |   |        |
|  | C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
|  | C <sub>6</sub> H <sub>6</sub>                 | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
|  | C <sub>6</sub> H <sub>6</sub>                 | (2-9) × 10 <sup>-3</sup>  |                   |                             |                             | 1.9                  | CP/Ac-14,38 | A = DPBF; λ <sub>exc</sub> = 578 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, ϕ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> = 0.024.   | 84F197 |
|  | CCl <sub>4</sub>                              | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
|  | CHCl <sub>3</sub>                             | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
|  | CS <sub>2</sub>                               | (1-50) × 10 <sup>-4</sup> |                   | -1                          | -1                          |                      | CP/Ac-14,38 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 767570 |
| <b>1.216 1,3,5-Hexatriene, 1,6-diphenyl- (DPH)</b>   |   |                           |                   |                             |                             |                      |             |   |        |
|  | c-C <sub>6</sub> H <sub>12</sub>              | air                       |                   |                             |                             |                      | PL/Ad-49,39 | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 5 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 3.4 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ε <sub>T</sub> (AC) = 114000 L mol <sup>-1</sup> cm <sup>-1</sup> at 416 nm. ϕ <sub>T</sub> ≈ 0; f <sub>Δ</sub> <sup>S</sup> + f <sub>T</sub> <sup>O<sub>2</sub></sup> f <sub>Δ</sub> <sup>T</sup> = 1.7. | 85F041 |
|  | n-C <sub>6</sub> H <sub>14</sub>              | O <sub>2</sub>            | 1.0               | ≥0.24                       | ≥0.17                       |                      | CP/Ac-27    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used p <sub>A</sub> = 1.  | 79E643 |
|  | MeOH  | air                       |                   |                             |                             |                      | PL/Ad-49,39 | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 1 × 10 <sup>5</sup> s <sup>-1</sup> , k <sub>A</sub> = 8 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ε <sub>T</sub> (AC) = 121000 L mol <sup>-1</sup> cm <sup>-1</sup> at 410 nm. ϕ <sub>T</sub> ≈ 0; f <sub>Δ</sub> <sup>S</sup> + f <sub>T</sub> <sup>O<sub>2</sub></sup> f <sub>Δ</sub> <sup>T</sup> = 1.6.   | 85F041 |
| <b>1.217 Indole, 1-methyl-</b>   |   |                           |                   |                             |                             |                      |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>          |                   | 0.35                        |                             |                      | PL/βCb-57   | S' = BP; TD = AP; rel. to ϕ <sub>Δ</sub> (S') = 0.35. Measured f <sub>Δ</sub> <sup>T</sup> (S)/ϕ <sub>Δ</sub> (S') = 1.0.   | 76F904 |
|  | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>          |                   | >0.2                        |                             |                      | PL/βCb-57   | S' = BP; TD = Xanthone; rel. to ϕ <sub>Δ</sub> (S') = 0.35. Measured f <sub>Δ</sub> <sup>T</sup> (S)/ϕ <sub>Δ</sub> (S') = 0.7 but energy transfer efficiency < 100%.   | 76F904 |
| <b>1.218 β-Ionone</b>  |   |                           |                   |                             |                             |                      |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>            | 0.22 <sup>*</sup> | 0.25 <sup>T</sup>           | -0.5                        |                      | PL/Ad-43,39 | S' = BP; A = DPBF; rel. to ϕ <sub>Δ</sub> (S') = 0.4; meas. ϕ <sub>T</sub> (S) = 0.5; λ <sub>exc</sub> = 337 nm.  | 85E293 |
| <b>1.219 Isobenzofuran, 1,3-diphenyl- (DPBF)</b>   |   |                           |                   |                             |                             |                      |             |   |        |
|  | c-C <sub>6</sub> H <sub>12</sub>              | air <sup>a</sup>          | 0.22              |                             |                             |                      | CP/Ac-14    | A = S; λ <sub>exc</sub> = 365 nm. In presence of 5 g L <sup>-1</sup> ethylene-propylene-ethylidene-norbornene terpolymer.   | 84P629 |
|  | C <sub>6</sub> H <sub>6</sub>                 | air                       | 0.26              |                             |                             |                      | CP/Ac-14    | A = S; λ <sub>exc</sub> = 365 nm.   | 81F017 |
|  | C <sub>6</sub> H <sub>6</sub>                 | 1.9 × 10 <sup>-3</sup>    | 0.28              |                             |                             |                      | CP/Ac-46    | A = S; λ <sub>exc</sub> = 365 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured ϕ <sub>Δ</sub> (S)/ϕ <sub>Δ</sub> (S') = 0.30 and 0.56 for S' = Cor and BP, resp.   | 81F364 |
|  | C <sub>6</sub> H <sub>6</sub>                 | 9.0 × 10 <sup>-3</sup>    | 0.78              |                             |                             | 1.5                  | CP/Ac-46    | A = S; λ <sub>exc</sub> = 365 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured ϕ <sub>Δ</sub> (S)/ϕ <sub>Δ</sub> (S') = 0.80 and 0.88 for S' = Cor and BP, resp.   | 81F364 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                          | [O <sub>2</sub> ]            | Φ <sub>Δ</sub>   | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.   |
|--|----------------------------------|------------------------------|------------------|-----------------------------|-----------------------------|----------------------|-------------|---|--------|
| <b>1.220 Naphthalene (Np)</b>                      |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | Hexanes                          | O <sub>2</sub>               | 0.73             |                             |                             |                      | CP/Ac-14    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm. Independent of concentration.   | 78F016 |
|  | c-C <sub>6</sub> H <sub>12</sub> | air                          |                  | 1.0                         |                             |                      | PL/Ad,St-49 | A = DPBF; AC = S; TD = p-MAP; λ <sub>exc</sub> = 355 nm; used k <sub>d</sub> = 4.2 × 10 <sup>4</sup> s <sup>-1</sup> , ε <sub>T(S)</sub> = 24,500 L mol <sup>-1</sup> cm <sup>-1</sup> at 415 nm.   | 87E234 |
|  | n-C <sub>6</sub> H <sub>14</sub> | air                          | 0.5              |                             |                             |                      | PL/Ad-43    | S' = An; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 264 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 82E258 |
|  | C <sub>6</sub> D <sub>6</sub>    | air                          |                  | 0.59*                       | 0.49                        |                      | PR/LI-60    | S' = BP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.29.   | 89E113 |
|  | C <sub>6</sub> H <sub>6</sub>    | air or O <sub>2</sub>        |                  | 0.62                        |                             |                      |             | See Table 4.  |        |
|  | C <sub>6</sub> H <sub>6</sub>    | air                          | 0.68*            | 0.56                        |                             |                      | PR/βCb-59   | S' = BP; TA = Car; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.29; used ε <sub>T(S)</sub> = 13,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 425 nm, ε <sub>T(S)</sub> = 7630 L mol <sup>-1</sup> cm <sup>-1</sup> at 532.5 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> > 0.94.                | 89E158 |
|  | C <sub>6</sub> H <sub>6</sub>    | air                          |                  | 0.55                        |                             |                      | PL/Ad,St-49 | A = DPBF; TD = p-MAP; λ <sub>exc</sub> = 355 nm; used k <sub>d</sub> = 3.1 × 10 <sup>4</sup> s <sup>-1</sup> , ε <sub>T(S)</sub> = 13,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 425 nm.   | 87E234 |
|  | C <sub>6</sub> H <sub>6</sub>    | air <sup>a</sup>             |                  | 0.65                        |                             |                      | PL/βCb-57   | S' = BP; TD = AP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.35. Measured f <sub>Δ</sub> <sup>T</sup> (S)/f <sub>Δ</sub> <sup>T</sup> (S') = 1.9.   | 76F904 |
|  | C <sub>6</sub> H <sub>6</sub>    | air <sup>a</sup>             |                  | 0.60                        |                             |                      | PL/βCb-57   | S' = BP; TD = Xanthone; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.35. Measured f <sub>Δ</sub> <sup>T</sup> (S)/f <sub>Δ</sub> <sup>T</sup> (S') = 1.7.   | 76F904 |
|  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>               |                  | 0.5                         |                             |                      | PR/Ad,St-49 | A = DPBF; used ϕ <sub>T(S)</sub> = 0.82, ε <sub>T(S)</sub> = 13,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 425 nm. Measured G( <sup>3</sup> S*).   | 78E263 |
|  | D <sub>2</sub> O (mic)           | O <sub>2</sub>               |                  | 1.0                         |                             |                      | PL/Ad-49    | A = DPBF; TD = BP; λ <sub>exc</sub> = 355 nm; used k <sub>d</sub> = 2.4 × 10 <sup>4</sup> s <sup>-1</sup> . Soln. cont. 0.2–0.5 mol L <sup>-1</sup> SDS; ε <sub>T(S)</sub> detd. in SDS at 415 nm by comparison with ε = 24500 L mol <sup>-1</sup> cm <sup>-1</sup> at 415 nm in cyclohexane. | 87E234 |
|  | MeOH                             | O <sub>2</sub>               | 0.41             |                             |                             |                      | CP/Ac-14    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; P <sub>S</sub> <sup>O<sub>2</sub></sup> = P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; [S] → 0.  | 78F016 |
|  | MeOH                             | O <sub>2</sub>               | 0.14             |                             |                             |                      | CP/Oc-14    | A = TME; λ <sub>exc</sub> = 283–373 nm.   | 70F735 |
|  | MeOH                             | O <sub>2</sub>               | 0.14             |                             |                             |                      | CP/Oc-14    | A = 2,5-DMF; λ <sub>exc</sub> = 283–373 nm.   | 70F735 |
| <b>1.221 Naphthalene excimer</b>                   |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | MeOH                             | O <sub>2</sub>               | 0.89             |                             |                             |                      | CP/Ac-14    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm. Assumed f <sub>Δ</sub> <sup>T</sup> = 1; [S] → ∞.   | 78F016 |
| <b>1.222 Naphthalene, 1-bromo-</b>                 |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | MeOH                             | O <sub>2</sub>               | 0.86             |                             |                             |                      | CP/Ac-14    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm.   | 78F016 |
| <b>1.223 Naphthalene, 1-methyl- (1MN)</b>          |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | c-C <sub>6</sub> H <sub>12</sub> | → ∞                          |                  | 0.77 <sup>ST</sup>          |                             |                      | PL/LI-56    | S' = Py; rel. to Φ <sub>Δ</sub> (S') = 0.81; λ <sub>exc</sub> = 355 nm.   | 91E297 |
|  | CH <sub>3</sub> CN               | → ∞                          |                  | 0.30 <sup>ST</sup>          |                             |                      | PL/LI-56    | S' = DCA; rel. to Φ <sub>Δ</sub> (S') = 2.0; λ <sub>exc</sub> = 355 nm.   | 91E297 |
| <b>1.224 2-Naphthalenethione, 1,1-dimethyl-</b>    |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>    | (1.9–9.1) × 10 <sup>-3</sup> | 0.6*             | 0.7 <sup>T</sup>            | 0.7                         |                      | PL/Ad-43,39 | S' = BP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.4; meas. ϕ <sub>T(S)</sub> = 1; λ <sub>exc</sub> = 337 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 86A240 |
|  | C <sub>6</sub> H <sub>6</sub>    | (1.9–9.1) × 10 <sup>-3</sup> | 1.0 <sup>T</sup> | 1.0                         |                             |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. ϕ <sub>T(S)</sub> = 1; λ <sub>exc</sub> = 532 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.  | 86A240 |
| <b>1.225 2-Naphthalenethione, 1,1,3-trimethyl-</b> |                                  |                              |                  |                             |                             |                      |             |   |        |
|  | C <sub>6</sub> H <sub>6</sub>    | (1.9–9.1) × 10 <sup>-3</sup> | 1.0 <sup>T</sup> | 1.0                         |                             |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. ϕ <sub>T(S)</sub> = 1; λ <sub>exc</sub> = 532 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.  | 86A240 |
|  | C <sub>6</sub> H <sub>6</sub>    | (1.9–9.1) × 10 <sup>-3</sup> | 0.7*             | 0.8 <sup>T</sup>            | 0.8                         |                      | PL/Ad-43,39 | S' = BP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.4; meas. ϕ <sub>T(S)</sub> = 1; λ <sub>exc</sub> = 337 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 86A240 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                          | [O <sub>2</sub> ]     | $\phi_{\Delta}$            | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.   |
|--|----------------------------------|-----------------------|----------------------------|-------------------|----------------|----------------------------|-------------|--|--------|
| <b>1.226 Norharman (<math>\beta</math>-Carboline)</b>  |                                  |                       |                            |                   |                |                            |             |  |        |
|  | D <sub>2</sub> O pD = 7          | air                   |                            | 0.03              |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.30$ ; $\lambda_{exc} = 337$ nm.   | 87F290 |
| <b>1.227 1,3,5,7-Octatetraene, 1,8-diphenyl- (DPO)</b>   |                                  |                       |                            |                   |                |                            |             |  |        |
|  | c-C <sub>6</sub> H <sub>12</sub> | air                   |                            |                   | 1.9            |                            | PL/Ad-49,39 | A = DPBF; AC = S; $\lambda_{exc} = 337$ nm; used $k_d = 5 \times 10^4$ s <sup>-1</sup> , $k_A = 3.4 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\epsilon_T(AC) = 210000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 437 nm.<br>$\phi_T \approx 0$ ; $f_{\Delta}^S + f_T^O f_{\Delta}^T = 1.9$ . | 85F041 |
|  | MeOH                             | air                   |                            |                   | 1.4            |                            | PL/Ad-49,39 | A = DPBF; AC = S; $\lambda_{exc} = 337$ nm; used $k_d = 1 \times 10^5$ s <sup>-1</sup> , $k_A = 3.4 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\epsilon_T(AC) = 191000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 430 nm.<br>$\phi_T \approx 0$ ; $f_{\Delta}^S + f_T^O f_{\Delta}^T = 1.4$ . | 85F041 |
| <b>1.228 2,4,6-Octatriene, 2,6-dimethyl- (Neoalloocimene)</b>  |                                  |                       |                            |                   |                |                            |             |  |        |
|  | C <sub>6</sub> H <sub>6</sub>    |                       | $1 \times 10^{-2}$         |                   | 0.54*          |                            | PL/LI-60    | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm.  | 89A235 |
|  |                                  |                       |                            |                   | 0.45           |                            |             | Measured $P_T^{O_2}$ .   |        |
| <b>1.229 3-Pentanethione, 2,2,4,4-tetramethyl- (DTBTK)</b>   |                                  |                       |                            |                   |                |                            |             |  |        |
|  | C <sub>6</sub> H <sub>6</sub>    |                       | $(1.9-9.1) \times 10^{-3}$ | 0.81 <sup>T</sup> | 0.85           |                            | PL/Ad-49,39 | A = DPBF; AC = DPH; TA = DPH; meas. $\phi_T(S) = 0.95^e$ ; $\lambda_{exc} = 490$ nm; used $k_d = 4.0 \times 10^4$ s <sup>-1</sup> , $k_A = 8.0 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 100,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 426 nm.      | 85A300 |
| <b>1.230 2-Pentanone</b>   |                                  |                       |                            |                   |                |                            |             |  |        |
|  | neat                             | O <sub>2</sub>        |                            | 0.03              |                |                            | CP/Ac-14    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. Used $p_A = 1$ .  | 79F184 |
| <b>1.231 3-Pentanone</b>   |                                  |                       |                            |                   |                |                            |             |  |        |
|  | neat                             | O <sub>2</sub>        |                            | 0.04              |                |                            | CP/Ac-14    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. Used $p_A = 1$ .  | 79F184 |
| <b>1.232 3-Pentanone, 2,4-dimethyl-</b>  |                                  |                       |                            |                   |                |                            |             |  |        |
|  | neat                             | O <sub>2</sub>        |                            | <0.0003           |                |                            | CP/Ac-14    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm. Used $p_A = 1$ .  | 79F184 |
| <b>1.233 Perylene (Per)</b>  |                                  |                       |                            |                   |                |                            |             |  |        |
|  | n-C <sub>6</sub> H <sub>14</sub> | O <sub>2</sub>        |                            | 1.3               | $\geq 0.65$    | $\geq 0.65$                | CP/Ac-27    | A = 2,5-DMF; $\lambda_{exc} = 366$ nm. $P_T^{O_2} = 1$ ; assumes $f_T^{O_2} = 1$ ; used $p_A = 1$ .  | 79E643 |
|  | C <sub>6</sub> H <sub>6</sub>    | air                   |                            |                   | 0.88*          |                            | PL/LI-60    | $S' = BP$ ; TD = BP; rel. to $f_{\Delta}^T(S') = 0.31$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ , cor. for energy transfer efficiency.  | 90A328 |
|  | C <sub>6</sub> H <sub>6</sub>    | air                   |                            |                   | 0.29           |                            | PL/LI-56    | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$ ; Assumed $f_T^{O_2} = 1$ .   | 90A328 |
|  | C <sub>6</sub> H <sub>6</sub>    | var.                  |                            |                   |                | 0.56                       | PL/LI-38,56 | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = -0. P_T^{O_2} = 1$ ; Assumed $f_T^{O_2} = 1$ , used $f_{\Delta}^T = 0.78$ .   | 90A328 |
|  | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub> var.   |                            |                   | ~1             |                            | CP/Ac-14,38 | $\lambda_{exc} = 435.8$ nm. A = DMA and DMBA; results consistent with $f_{\Delta}^S \ll f_{\Delta}^T$ ; assumed $f_T^{O_2} = 1$ ; meas. $\phi_{\Delta}^T(f_{\Delta}^T + f_{\Delta}^S) = 0.06$ .  | 69F388 |
| <b>1.234 Perylo[1,12-def]-1,3-dioxepin-5,11-dione, 6,12-dihydroxy-8,9-bis(2-hydroxypropyl)-7,10-dimethoxy- (Cercosporin)</b> |                                  |                       |                            |                   |                |                            |             |  |        |
|  | C <sub>6</sub> D <sub>6</sub>    | air or O <sub>2</sub> |                            | 0.81              |                |                            | PL/LI-56    | $S' = MPDME$ ; rel. to $\phi_{\Delta}(S') = 0.81$ ; $\lambda_{exc} = 532$ nm.  | 83R123 |
|  | C <sub>6</sub> D <sub>6</sub>    | air <sup>a</sup>      |                            | 0.81              |                |                            | CP/Ac-43    | $S' = MPDME$ ; A = 2M2P; rel. to $\phi_{\Delta}(S') = 0.81$ .  | 83R123 |
| <b>1.235 Phenalen-1-one</b>  |                                  |                       |                            |                   |                |                            |             |  |        |
|  | C <sub>6</sub> D <sub>6</sub>    | air <sup>a</sup>      |                            | 0.94 <sup>T</sup> | 0.95           |                            | CP/LI-56,42 | $S' = 9$ -Fluorenone; rel. to $\phi_{\Delta}(S') = 0.83$ ; meas. $\phi_T(S) = 1.0^d$ ; $\lambda_{exc} = 367$ nm; used $\phi_T(S) = 1^d$ . Assumed $P_T^{O_2} = 1$ .  | 91F023 |
|  | C <sub>6</sub> H <sub>6</sub>    | air <sup>a</sup>      |                            | 0.93 <sup>T</sup> | 0.93           |                            | CP/LI-56,42 | $S' = 9$ -Fluorenone; rel. to $\phi_{\Delta}(S') = 0.83$ ; meas. $\phi_T(S) = 1.0$ ; $\lambda_{exc} = 367$ nm. Assumed $P_T^{O_2} = 1$ .   | 91F023 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]     | $\phi_{\Delta}$   | $f_{\Delta}^T$     | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment   | Ref.   |
|---|---|-----------------------|-------------------|--------------------|----------------|----------------------------|-------------|---|--------|
| <b>1.235 Phenalen-1-one—Continued</b>   |   |                       |                   |                    |                |                            |             |   |        |
|   | CCl <sub>4</sub>                              | air <sup>a</sup>      |                   | 0.95 <sup>T</sup>  |                |                            | CP/Ac-14    | A = TME. D.E. Nicodem, R.S. da Silva, M.M. da Silva, personal communication.  | 91F023 |
|   | CD <sub>3</sub> OD                            | air <sup>a</sup>      |                   | 0.97 <sup>T</sup>  | 0.97           |                            | CP/LI-56,42 | S' = RB; rel. to $\phi_{\Delta}(S') = 0.76$ ; meas. $\phi_T(S) = 1.0$ . $P_T^{O_2} = 1$ ; meas. ratio of $I_a$ at $\lambda_{exc}(S) = 367$ and $\lambda_{exc}(S') = 547$ nm.  | 91F023 |
| <b>1.236 Phenalen-1-one, 6-amino-</b>   |   |                       |                   |                    |                |                            |             |   |        |
|   | EtOH  | air <sup>a</sup>      |                   | 0.043              |                |                            | CP/Ac-14    | A = DMA. Extrapolated to [DMA] → ∞.   | 85F501 |
| <b>1.237 Phenanthrene</b>   |   |                       |                   |                    |                |                            |             |   |        |
|   | c-C <sub>6</sub> H <sub>12</sub>              | → ∞                   |                   | 0.44 <sup>ST</sup> |                |                            | PL/LI-56    | S' = Py; rel. to $\phi_{\Delta}(S') = 0.81$ ; $\lambda_{exc} = 355$ nm.   | 91E297 |
|   | n-C <sub>6</sub> H <sub>14</sub>              | air                   |                   | 0.3 <sup>T</sup>   |                |                            | PL/Ad-43    | S' = An; A = DPBF; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 264$ nm. $P_T^{O_2} = 1$ .  | 82E258 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.59              | 0.84               |                |                            | PL/Hp-52,42 | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.70$ . Measured $\phi_{\Delta} = 0.57$ , $P_T^{O_2} = 0.97$ and $\phi_F$ .   | 88E449 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.62              | 0.88               |                |                            | PL/LI-56,42 | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 0.70$ . Measured $P_T^{O_2} = 0.97$ .   | 88E449 |
|   | CH <sub>3</sub> CN                            | → ∞                   |                   | 0.24 <sup>ST</sup> |                |                            | PL/LI-56    | S' = DCA; rel. to $\phi_{\Delta}(S') = 2.0$ ; $\lambda_{exc} = 355$ nm.   | 91E297 |
|   | MeOH  | O <sub>2</sub>        | 0.50              |                    |                |                            | CP/Ac-14    | A = 2,5-DMF; $\lambda_{exc} = 313$ nm.  | 78F016 |
| <b>1.238 Phenanthro[1,10,9,8-opqua]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (Hypericin, HYP)</b> |   |                       |                   |                    |                |                            |             |   |        |
|   | D <sub>2</sub> O (mic)                        | air                   | 0.72              | 1                  |                |                            | PL/Ad-49,42 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.70$ ; $\lambda_{exc} = 640$ nm; used $k_d = 2.0 \times 10^4$ s <sup>-1</sup> , $k_A = 1.0 \times 10^9$ L mol <sup>-1</sup> s <sup>-1</sup> , $\varepsilon_T(AC) = 19400$ L mol <sup>-1</sup> cm <sup>-1</sup> at 640 nm. BRJ 35 micelles.                    | 88N343 |
|   | pH = ~7                                       |                       |                   |                    |                |                            |             |   |        |
|   | EtOH  | $2.1 \times 10^{-3}$  | 0.73              | 1                  | 0              |                            | PL/Ad-49,39 | A = MDH; P = Mesodiphenylhelianthrene endoperoxide; AC = S; $\lambda_{exc} = 308$ nm; used $k_d = 8.3 \times 10^4$ s <sup>-1</sup> , $k_A = 7.0 \times 10^9$ L mol <sup>-1</sup> s <sup>-1</sup> , $\phi_T(S) = 0.71$ , $\varepsilon_T(AC) = 13100$ L mol <sup>-1</sup> cm <sup>-1</sup> at 630 nm. | 87F541 |
| <b>1.239 Phenazine (Pz)</b>   |   |                       |                   |                    |                |                            |             |   |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air or O <sub>2</sub> | 0.88              | 1.0                |                |                            |             | See Table 4.  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                   | 0.83 <sup>T</sup> | 0.98               |                |                            | PL/LI-57,42 | used $\phi_T(S) = 0.85$ . S' = Pz in O <sub>2</sub> , $\phi_{\Delta}(S') = 0.83$ ; $P_T^{O_2} = 1$ .  | 90A328 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>        | 0.83 <sup>T</sup> | 0.98               |                |                            | PL/Hp-52,42 | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0.85$ . Measured $\phi_{\Delta} = 0.83$ , $P_T^{O_2} = 1$ and $\phi_F$ .  | 88E449 |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>        | 0.89 <sup>T</sup> |                    |                |                            | PL/Hp-52    | $\lambda_{exc} = 354$ nm.   | 88Z155 |
|   | CHCl <sub>3</sub>                             | O <sub>2</sub>        | 0.84 <sup>T</sup> |                    |                |                            | PL/Hp-52    | $\lambda_{exc} = 354$ nm.   | 88Z155 |
|   | i-octane/<br>H <sub>2</sub> O (96:4)<br>(mic) | O <sub>2</sub>        | 0.80              |                    |                |                            | PL/Hp-53    | $\lambda_{exc} = 355$ nm. Soln. cont. 0.1 mol L <sup>-1</sup> AOT; meas. $\phi_F = <0.01$ .   | 91N191 |
| <b>1.240 Phenothiazine</b>  |   |                       |                   |                    |                |                            |             |   |        |
|   | CH <sub>3</sub> CN                            | O <sub>2</sub>        | 0.20              | 0.21               |                |                            | PL/LI-56,42 | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; meas. $\phi_T(S) = 0.96^f$ ; $\lambda_{exc} = 355$ nm.  | 91A308 |
| <b>1.241 Phenothiazine, 2-acetyl-</b>   |   |                       |                   |                    |                |                            |             |   |        |
|   | CH <sub>3</sub> CN                            | O <sub>2</sub>        | ~0.46             |                    |                |                            | PL/LI-56    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 355$ nm.   | 91A308 |
| <b>1.242 Phenothiazine, 2-methoxy-</b>  |   |                       |                   |                    |                |                            |             |   |        |
|   | CH <sub>3</sub> CN                            | O <sub>2</sub>        | 0.21              |                    |                |                            | PL/LI-56    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 355$ nm.   | 91A308 |
| <b>1.243 Phenothiazine, 10-methyl-</b>  |   |                       |                   |                    |                |                            |             |   |        |
|   | CH <sub>3</sub> CN                            | O <sub>2</sub>        | 0.19              |                    |                |                            | PL/LI-56    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 355$ nm.   | 91A308 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]      | ϕ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment   | Ref.             |
|--|--|------------------------|-------------------|-----------------------------|-----------------------------|----------------------|-------------|---|------------------|
| <b>1.244 Phenothiazine, 2-(trifluoromethyl)-</b>                           |  |                        |                   |                             |                             |                      |             |   |                  |
|  | CH <sub>3</sub> CN   | O <sub>2</sub>         | 0.18              |                             |                             |                      | PL/LI-56    | S' = Pz; rel. to ϕ <sub>Δ</sub> (S') = 0.83; λ <sub>exc</sub> = 355 nm.   | 91A308           |
| <b>1.245 Phenothiazinium, 3,7-bis(dimethylamino)- (Methylene Blue, MB)</b> |  |                        |                   |                             |                             |                      |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH                 | air                    | 0.48 <sup>T</sup> |                             |                             |                      | CP/Ac-14    | A = DPBF. [O <sub>2</sub> ] varied.   | 87F479           |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> / MeOH<br>(99:1)   | air                    | 0.51 <sup>T</sup> |                             |                             |                      | CP/Ac-14    | A = DPBF. [O <sub>2</sub> ] varied.   | 87F479           |
|  | CH <sub>2</sub> Cl <sub>2</sub>                                  | air <sup>a</sup>       | 0.57 <sup>T</sup> | ~1                          |                             |                      | CP/Ac-14,42 | A = 2,5-DMF; used ϕ <sub>T</sub> (S) = 0.52. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 737339           |
|  | CH <sub>3</sub> CN   | air                    | 0.52 <sup>T</sup> |                             |                             |                      | CP/Pa-14    | A = DPF; P = 2,5-Diphenylfuran endoperoxide. Method adapted to allow for chain reaction.  | 87F440           |
|  | EtOH   | air <sup>a</sup>       | 0.52 <sup>T</sup> | 1                           |                             |                      | CP/Ac-14,42 | A = DMA; used ϕ <sub>T</sub> (S) = 0.52. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 737339           |
|  | EtOH   | 9.9 × 10 <sup>-3</sup> | 0.50 <sup>T</sup> | ~1                          |                             |                      | CP/Oc-43,39 | A = TME; rel. to ϕ <sub>Δ</sub> (S') = 0.50; used ϕ <sub>T</sub> (S) = 0.52 <sup>f</sup> . Used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to MB <sup>+</sup> in MeOH.   | 84F191           |
|  | H <sub>2</sub> O   | air                    | 0.60 <sup>T</sup> |                             |                             |                      | CP/Ac-27    | A = 2,5-DMF. Assumed f <sub>r</sub> <sup>A</sup> = 2; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 78F061           |
|  | H <sub>2</sub> O   | air <sup>a</sup>       | 0.52 <sup>T</sup> | 1                           |                             |                      | CP/Ac-14,42 | A = 2,5-DMF; used ϕ <sub>T</sub> (S) = 0.52. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 737339           |
|  | H <sub>2</sub> O<br>pH = 7.4                                     | O <sub>2</sub>         | 0.39 <sup>T</sup> |                             |                             |                      | CP/Ac-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to ϕ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.  | 85R008           |
|  | H <sub>2</sub> O (mic)<br>pH = 7.4                               | O <sub>2</sub>         | 0.37 <sup>T</sup> |                             |                             |                      | CP/Ac-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to ϕ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 546 nm. RNO as monitor of P; 0.23 mg/mL egg phosphatidylcholine.  | 85R008           |
|  | MeOD   | ~10 <sup>-3</sup>      | 0.70*             |                             |                             |                      | PL/LI-56    | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.57; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in EtOH; recalcd. using ϕ <sub>Δ</sub> (S') = 0.64 [88Z155]. | 88A165           |
|  | MeOH   | air                    | 0.50 <sup>T</sup> |                             |                             |                      | CP/Ac-14    | A = DPBF.   | 90F157           |
|  | MeOH   | air <sup>a</sup>       | 0.57 <sup>T</sup> |                             |                             |                      | PL/LI-56    | S' = Ery; rel. to ϕ <sub>Δ</sub> (S') = 0.60.   | 87R138           |
|  | MeOH   | air <sup>a</sup>       | 0.52 <sup>T</sup> |                             |                             |                      | CP/Ac-14,42 | A = DPBF; used ϕ <sub>T</sub> (S) = 0.52. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 737339           |
|  | MeOH   | O <sub>2</sub>         | 0.52 <sup>T</sup> |                             |                             |                      | CL/Ac-14    | A = DPBF; λ <sub>exc</sub> = 633 nm. Assumed f <sub>Δ</sub> <sup>T</sup> = 1.   | 87E690           |
|  | MeOH/<br>C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub><br>(97:3) | air                    | 0.48 <sup>T</sup> |                             |                             |                      | CP/Ac-14    | A = DPBF. [O <sub>2</sub> ] varied.   | 87F479           |
|  | 2-Methoxy- ethanol   | O <sub>2</sub>         | 0.43 <sup>T</sup> |                             |                             |                      | CL/Ac-14    | A = DPBF; λ <sub>exc</sub> = 633 nm. Assumed f <sub>Δ</sub> <sup>T</sup> = 1.   | 87E690           |
|  | Propylene carbonate  | O <sub>2</sub>         | 0.35 <sup>T</sup> |                             |                             |                      | CL/Ac-14    | A = DPBF; λ <sub>exc</sub> = 633 nm. Assumed f <sub>Δ</sub> <sup>T</sup> = 1.   | 87E690           |
| <b>1.246 Phenothiazinium, 3,7-diamino- (Thionine)</b>                      |  |                        |                   |                             |                             |                      |             |   |                  |
|  | CH <sub>3</sub> CN   | air                    | 0.58 <sup>T</sup> |                             |                             |                      | CP/Pa-14    | A = DPF; P = 2,5-Diphenylfuran endoperoxide. Method adapted to allow for chain reaction.  | 87F440           |
|  | H <sub>2</sub> O   | air <sup>a</sup>       | 0.58 <sup>T</sup> | 1                           |                             |                      | CP/Ac-43,42 | S' = MB <sup>+</sup> ; A = 2,5-DMF; rel. to ϕ <sub>Δ</sub> (S') = 0.52; used ϕ <sub>T</sub> (S) = 0.55. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 737339           |
| <b>1.247 Pivalothiophenone</b>   |  |                        |                   |                             |                             |                      |             |   |                  |
|  | C <sub>6</sub> H <sub>6</sub>                                    | air                    | 1.0 <sup>T</sup>  | 1.0                         |                             |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to ϕ <sub>Δ</sub> (S') = 1; meas. ϕ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 532 nm.   | 87A340           |
|  | CHCl <sub>3</sub>  | air <sup>a</sup>       | 1.0 <sup>T</sup>  | 1.0                         |                             |                      | CP/Ac-14,42 | A = DTBF; used ϕ <sub>T</sub> (S) = 1. [S] → 0, ϕ <sub>Δ</sub> = 0.94 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment  | Ref.             |
|-------|---|-------------------|----------------|-----------------------------|-----------------------------|----------------------|-------------|--|------------------|
| 1.248 | Pivalothiophenone, 4'-chloro-                               |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | air <sup>a</sup>  |                | 1.1 <sup>T</sup>            | 1                           |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. Φ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 532 nm.  | 87A340           |
| 1.249 | Pivalothiophenone, 4'-fluoro-                               |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | air               |                | 0.98 <sup>T</sup>           | 0.98                        |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. Φ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 532 nm.  | 87A340           |
| 1.250 | Pivalothiophenone, 4'-methoxy-                              |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | air               |                | 0.87 <sup>T</sup>           | 0.87                        |                      | PL/Ad-43,39 | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. Φ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 532 nm.  | 87A340           |
|       | CHCl <sub>3</sub>   | air <sup>a</sup>  |                | 1.0 <sup>T</sup>            | 1.0                         |                      | CP/Ac-14,42 | A = DTBF; used Φ <sub>T</sub> (S) = 1. [S] → 0, Φ <sub>Δ</sub> = 0.86 at [S] = 0.01 mol L <sup>-1</sup> .  | 83F028<br>82F140 |
| 1.251 | 1,2-Propanedione, 1-phenyl-                                 |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.38                        |                             |                      | CP/Pa-14    | A = 1,2-Dimethylcyclohexene; λ <sub>exc</sub> = 366 nm. P = 3-Hydroxy-1,2-dimethylcyclohexene, 2-Hydroxy-2-methyl-1-methylenecyclohexane, and 3-Hydroxy-2,3-dimethylcyclohexene.   | 85F153           |
| 1.252 | Pseudoisopsoralen (Furo[3,2- <i>h</i> ][1]benzopyran-8-one) |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.01 <sup>T</sup>           | 0.33                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.03; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121           |
| 1.253 | Pseudopsoralen (Furo[2,3- <i>g</i> ][1]benzopyran-6-one)    |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.03 <sup>T</sup>           | 0.60                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.05; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121<br>86E160 |
| 1.254 | Pseudopsoralen, 3-carbethoxy-                               |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.56*                       |                             |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.51; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121<br>86E160 |
|       |   |                   |                | 0.49 <sup>T</sup>           | 0.96                        |                      |             |  |                  |
| 1.255 | Psoralen (Furo[3,2- <i>g</i> ][1]benzopyran-7-one)          |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.01 <sup>T</sup>           | 0.33                        |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.03; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121<br>86E160 |
|       | CCl <sub>4</sub>  | air               |                | 0.0055                      |                             |                      | MP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 652 nm.  | 83E813           |
|       | D <sub>2</sub> O<br>pD = 7.0                                | O <sub>2</sub>    |                | 0.18                        |                             |                      | CP/Ac-44    | S' = HP; A = Subtilisin Carlsberg; rel. to Φ <sub>Δ</sub> (S') = 0.43; λ <sub>exc</sub> = 365 nm.  | 87R015           |
|       | D <sub>2</sub> O  | air               |                | 0.04                        |                             |                      | PL/LI-56    | S' = RF; rel. to Φ <sub>Δ</sub> (S') = 0.3; λ <sub>exc</sub> = 337 nm.   | 86E959<br>86F144 |
|       | MeOH  | air               |                | 0.05                        |                             |                      | PL/LI-56    | S' = RF; rel. to Φ <sub>Δ</sub> (S') = 0.4; λ <sub>exc</sub> = 337 nm.   | 86E959<br>86F144 |
| 1.256 | Psoralen, 3-carbethoxy-                                     |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.34*                       |                             |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.30; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121<br>86E160 |
|       |   |                   |                | 0.30 <sup>T</sup>           | 1.0                         |                      |             |  |                  |
|       | H <sub>2</sub> O<br>pH = 7.3                                | O <sub>2</sub>    |                | 0.3 <sup>T</sup>            | 1                           |                      | CP/Pa-43,42 | S' = Ang; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.02 <sup>b</sup> ; λ <sub>exc</sub> = 365 nm; used Φ <sub>T</sub> (S) = 0.32 <sup>d</sup> . RNO as monitor of P; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 84F111           |
| 1.257 | Psoralen, 5,8-dimethoxy-                                    |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | O <sub>2</sub>    |                | 0.005*                      |                             |                      | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.04; λ <sub>exc</sub> = 355 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 88E121<br>86E160 |
|       |   |                   |                | 0.004 <sup>T</sup>          | 0.10                        |                      |             |  |                  |
| 1.258 | Psoralen, 5-methoxy-  |                   |                |                             |                             |                      |             |  |                  |
|       | C <sub>6</sub> H <sub>6</sub>                               | air               |                | 0                           |                             |                      | PL/LI-56    | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.29; λ <sub>exc</sub> = 308 nm. No emission detected.  | 91F273           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ]                     | $\phi_{\Delta}$ | $f_{\Delta}^T$               | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method      | Comment  | Ref.             |
|--|---|---------------------------------------|-----------------|------------------------------|----------------|----------------------------|-------------|--|------------------|
| <b>1.258 Psoralen, 5-methoxy—Continued</b>     |   |                                       |                 |                              |                |                            |             |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        |                 | 0.02 <sup>T</sup>            | 0.29           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.07$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121<br>86E160 |
|  | D <sub>2</sub> O<br>pD $\leq 7.0$             | O <sub>2</sub>                        |                 | 0.013                        |                |                            | CP/Ac-44    | $S' = HP$ ; A = Subtilisin Carlsberg; rel. to $\phi_{\Delta}(S') = 0.43$ ; $\lambda_{exc} = 365$ nm.   | 87R015           |
| <b>1.259 Psoralen, 5-methoxy-, DNA complex</b> |   |                                       |                 |                              |                |                            |             |  |                  |
|  | D <sub>2</sub> O/EtOH<br>(97.5:2.5)           | O <sub>2</sub>                        |                 |                              |                |                            | CP/Ac-43    | $S' = 5\text{-MOP}$ ; A = DOPA; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 3.2$ ; $\lambda_{exc} = 313$ nm. Soln. contg. 0.1% DNA, $2 \times 10^{-3}$ mol L <sup>-1</sup> NaCl.                 | 81F482           |
|  | D <sub>2</sub> O/EtOH<br>(97.5:2.5)           | O <sub>2</sub>                        |                 |                              |                |                            | CP/Ac-43    | $S' = 5\text{-MOP}$ ; A = DOPA; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 3.6$ ; $\lambda_{exc} = 335$ nm. Soln. contg. 0.1% DNA, $2 \times 10^{-3}$ mol L <sup>-1</sup> NaCl.                 | 81F482           |
| <b>1.260 Psoralen, 8-methoxy- (8-MOP)</b>      |   |                                       |                 |                              |                |                            |             |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>                 | air                                   |                 | <0.02                        |                |                            | PL/LI-56    | $S' = BP$ ; rel. to $\phi_{\Delta}(S') = 0.29$ ; $\lambda_{exc} = 308$ nm. No emission detected.   | 91F273           |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        |                 | 0.005*<br>0.004 <sup>T</sup> | 0.4            |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.01$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121<br>86E160 |
|  | CCl <sub>4</sub>                              | air                                   |                 | 0.002 <sup>T</sup>           |                |                            | MP/LI-56    | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 652$ nm.   | 83E813           |
|  | CCl <sub>4</sub>                              | air <sup>a</sup>                      |                 | <0.03                        |                |                            | MP/LI-56    | $S' = An$ . Used $\phi_T(An) = 0.7$ .  | 82F071           |
|  | D <sub>2</sub> O<br>pD = 7.0                  | O <sub>2</sub>                        |                 | 0.035                        |                |                            | CP/Ac-44    | $S' = HP$ ; A = Subtilisin Carlsberg; rel. to $\phi_{\Delta}(S') = 0.43$ ; $\lambda_{exc} = 365$ nm.   | 87R015           |
|  | D <sub>2</sub> O                              | air                                   |                 | 0.009                        |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.3$ ; $\lambda_{exc} = 337$ nm.  | 86E959<br>86F144 |
|  | H <sub>2</sub> O                              | air                                   |                 | -0.0007                      |                |                            | CP/Ac-14    | $\Delta = S$ ; $\lambda_{exc} = 313$ nm.   | 83F188           |
|  | H <sub>2</sub> O/EtOH<br>(1:1)                | air <sup>a</sup>                      |                 | 0.03 <sup>T</sup>            |                |                            | PL/LI-56    | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.5$ ; $\lambda_{exc} = 337$ nm.  | 86F144           |
|  | MeOH  | air                                   |                 | 0.02 <sup>T</sup>            | ~0.7           |                            | PL/LI-56,42 | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.4$ ; $\lambda_{exc} = 337$ nm; used $\phi_T(S) = 0.03^d$ .  | 86E959<br>86F144 |
| <b>1.261 Psoralen, 4,5',8-trimethyl-</b>       |   |                                       |                 |                              |                |                            |             |  |                  |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        |                 | 0.09*<br>0.08 <sup>T</sup>   | 0.38           |                            | PL/LI-56,42 | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.21$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ .  | 88E121<br>86E160 |
| <b>1.262 Pyranthrene</b>                       |   |                                       |                 |                              |                |                            |             |  |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | $1.2 \times 10^{-3}$                  |                 |                              |                | 0.97                       | PL/Ad,St-48 | $A = Rub$ ; meas. $\phi_T(S) = 0.55$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ ; used $\epsilon_T(S) = 14,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at $\lambda_{max}$ ; $n_{\Delta} = 0.97$ . | 83F075           |
|  | C <sub>6</sub> H <sub>5</sub> CN              | $1.2 \times 10^{-3}$                  |                 |                              |                | 0.45                       | PL/Ad,St-48 | $A = Rub$ ; meas. $\phi_T(S) = 0.52$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ ; used $\epsilon_T(S) = 8,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at $\lambda_{max}$ ; $n_{\Delta} = 0.45$ .  | 83F075           |
| <b>1.263 Pyrene (Py)</b>                       |   |                                       |                 |                              |                |                            |             |  |                  |
|  | Hexanes                                       | O <sub>2</sub>                        |                 | 0.86                         |                |                            | CP/Ac-14    | $A = 2,5\text{-DMF}$ ; $\lambda_{exc} = 313$ nm.   | 78F016           |
|  | n-C <sub>6</sub> H <sub>14</sub>              | O <sub>2</sub>                        |                 | 0.79                         |                |                            | CP/Ac-27    | $A = 2,5\text{-DMF}$ ; $\lambda_{exc} = 313$ nm. $P_T^{O_2} = 1$ ; used $p_A = 1$ .  | 79E643           |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | $1.2 \times 10^{-3}$                  |                 | 1.9                          |                |                            | PL/LI-56    | $S' = PdMPDME$ ; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.   | 82E010           |
|  | C <sub>6</sub> D <sub>6</sub>                 | 1.2% O <sub>2</sub> in N <sub>2</sub> |                 |                              | 0.65           |                            | PR/LI-60    | $S' = Np$ ; TD = BP; rel. to $f_{\Delta}^T(S') = 0.55$ . $P_T^{O_2} = 1$ ; cor. for energy transfer efficiency.  | 90A328           |
|  | C <sub>6</sub> H <sub>6</sub>                 | air                                   |                 | 0.71                         |                |                            | PL/LI-56    | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$   | 90A328           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                          | [O <sub>2</sub> ]                        | $\phi_{\Delta}$    | $f_{\Delta}^T$     | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method       | Comment   | Ref.   |
|---|----------------------------------|--|--------------------|--------------------|----------------|----------------------------|--------------|---|--------|
| <b>1.263 Pyrene (Py)—Continued</b>                                    |                                  |  |                    |                    |                |                            |              |   |        |
|   | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>                           |                    | 0.74 <sup>ST</sup> |                |                            | PL/Hp-52     | $\lambda_{\text{exc}} = 355 \text{ nm}$ . Measured $\phi_{\Delta} = 0.74$ , $P_T^{O_2} = 1$ and $\phi_T^{O_2} = 0.96$ and $\phi_F$ . Authors assume $f_{\Delta}^S = 0$ and use $\phi_T(S) = 0.96$ to give $f_{\Delta}^T = 0.77$ but $P_S^{O_2} = 0.95$ so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable. | 88E449 |
|   | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>                           |                    | 0.74 <sup>ST</sup> |                |                            | PL/LI-56     | $S' = P_z$ ; rel. to $\phi_{\Delta}(S') = 0.83$ . Measured $P_T^{O_2} = 1$ and $\phi_T^{O_2} = 0.96$ . Authors assume $f_{\Delta}^S = 0$ and use $\phi_T(S) = 0.96$ to give $f_{\Delta}^T = 0.77$ but $P_S^{O_2} = 0.95$ so values of $f_{\Delta}^S$ and $f_{\Delta}^T$ are indeterminable.                               | 88E449 |
|   | C <sub>6</sub> H <sub>6</sub>    | var.                                     |                    |                    | 0.13           | 0.78                       | PL/LI-38,56  | $S' = P_z$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; meas. $\phi_T(S) = 0.29$ . $P_T^{O_2} = 1$ ; Assumed $f_T^{O_2} = 1$ , used $f_{\Delta}^T = 0.65$ .   | 90A328 |
|   | C <sub>6</sub> H <sub>6</sub>    | $1.9 \times 10^{-3}, 9.0 \times 10^{-3}$ | 1.5 <sup>ST</sup>  | -1                 | -0.5           | 1.5                        | CL/Ac-49,38  | $S' = A = \text{DMA}$ ; rel. to $\phi_{\Delta}(S') = 1.0$ . Assumed $f_T^{O_2} = 1$ .   | 83F116 |
|   | CH <sub>3</sub> CN               | $\rightarrow \infty$                     | 0.42 <sup>ST</sup> |                    |                |                            | PL/LI-56     | $S' = \text{DCA}$ ; rel. to $\phi_{\Delta}(S') = 2.0$ ; $\lambda_{\text{exc}} = 355 \text{ nm}$ .   | 91E297 |
|   | H <sub>2</sub> O (mic)           | O <sub>2</sub>                           | 0.9                |                    |                |                            | CP/Ac-14     | A = DPBF; $\lambda_{\text{exc}} = 338 \text{ nm}$ . [SDS] = 0.1 mol L <sup>-1</sup> .   | 78A174 |
|   | H <sub>2</sub> O (mic)           | O <sub>2</sub>                           | 1.0                |                    |                |                            | CP/Ac-14     | A = DPBF; $\lambda_{\text{exc}} = 338 \text{ nm}$ . [DTAC] = 0.1 mol L <sup>-1</sup> .  | 78A174 |
|   | MeOH                             | O <sub>2</sub>                           | 0.6                |                    |                |                            | CP/Ac-14     | A = DPBF; $\lambda_{\text{exc}} = 338 \text{ nm}$ .   | 78A174 |
|   | MeOH                             | O <sub>2</sub>                           | 0.76               |                    |                |                            | CP/Ac-14     | A = 2,5-DMF; $\lambda_{\text{exc}} = 313 \text{ nm}$ . Assumed $f_{\Delta}^T = 1$ ; [S] → 0.  | 78F016 |
|   | MeOH                             | O <sub>2</sub>                           | 0.60               |                    |                |                            | CP/Oc-14     | A = 2,5-DMF; $\lambda_{\text{exc}} = 283-373 \text{ nm}$ .  | 70F735 |
|   | MeOH                             | O <sub>2</sub>                           | 0.63               |                    |                |                            | CP/Oc-14     | A = TME; $\lambda_{\text{exc}} = 283-373 \text{ nm}$ .  | 70F735 |
| <b>1.264 Pyrene, excimer</b>  |                                  |  |                    |                    |                |                            |              |   |        |
|   | C <sub>6</sub> H <sub>6</sub>    | $1.9 \times 10^{-3}, 9.0 \times 10^{-3}$ | 0.8                |                    | 0.8            |                            | CL/Ac-49,38  | $S' = A = \text{DMA}$ ; rel. to $\phi_{\Delta}(S') = 1.0$ . Assumed $f_T^{O_2} = 1$ .   | 83F116 |
|   | MeOH                             | O <sub>2</sub>                           | 0.46               |                    |                |                            | CP/Ac-14     | A = 2,5-DMF; $\lambda_{\text{exc}} = 313 \text{ nm}$ . Assumed $f_{\Delta}^T = 1$ ; [S] → ∞.  | 78F016 |
| <b>1.265 1-Pyrenecarboxaldehyde</b>                                   |                                  |  |                    |                    |                |                            |              |   |        |
|   | c-C <sub>6</sub> H <sub>12</sub> | O <sub>2</sub>                           |                    | 0.87 <sup>T</sup>  | 1              |                            | PL/Ad-49,42  | A = DPBF; AC = BP; $\lambda_{\text{exc}} = 337 \text{ nm}$ ; used $k_d = 5.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 3.4 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\phi_T(S) = 0.78^f$ , $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7600 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 532 nm.                                    | 84F005 |
|   | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>                           |                    | 0.68 <sup>T</sup>  | 1              |                            | PL/Ad-49,42  | A = DPBF; AC = BP; $\lambda_{\text{exc}} = 337 \text{ nm}$ ; used $k_d = 4.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 8.0 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\phi_T(S) = 0.57^f$ , $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7600 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 532 nm.                                    | 84F005 |
| <b>1.266 Pyridine, 2,6-bis(2-thienyl)-</b>                            |                                  |  |                    |                    |                |                            |              |   |        |
|   | CDCl <sub>3</sub>                | $\sim 1.16 \times 10^{-2}$               | 0.53 <sup>T</sup>  |                    |                |                            | PL/Ad,AcI-49 | A = DPBF; AC = BP; $\lambda_{\text{exc}} = 337 \text{ nm}$ ; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 525 nm. $p_A = 1$ .  | 87E410 |
| <b>1.267 α-Quaterthienyl</b>  |                                  |  |                    |                    |                |                            |              |   |        |
|   | EtOH                             | O <sub>2</sub>                           |                    | -0.2 <sup>T</sup>  | -1             |                            | PL/Ac-14,42  | A = DPBF; meas. $\phi_T(S) = 0.20^f$ ; $\lambda_{\text{exc}} = 353 \text{ nm}$ . $P_T^{O_2} = 1$ , $p_A = 0.75$ .   | 85N020 |
| <b>1.268 Quinoline</b>  |                                  |  |                    |                    |                |                            |              |   |        |
|   | MeOH                             | O <sub>2</sub>                           |                    | 0.09               |                |                            | CP/Oc-14     | A = 2,5-DMF; $\lambda_{\text{exc}} = 283-373 \text{ nm}$ .  | 70F735 |
|   | MeOH                             | O <sub>2</sub>                           |                    | 0.10               |                |                            | CP/Oc-14     | A = TME; $\lambda_{\text{exc}} = 283-373 \text{ nm}$ .  | 70F735 |
| <b>1.269 Quinoline-2-carboxylic acid, 4-hydroxy- (Kynurenic acid)</b> |                                  |  |                    |                    |                |                            |              |   |        |
|   | D <sub>2</sub> O pD = 7          | air                                      |                    | 0.16               |                |                            | PL/LI-56     | $S' = RF$ ; rel. to $\phi_{\Delta}(S') = 0.30$ ; $\lambda_{\text{exc}} = 337 \text{ nm}$ .  | 87F290 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                          | [O <sub>2</sub> ]      | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment  | Ref.   |
|---|----------------------------------|------------------------|----------------|-----------------------------|-----------------------------|----------------------|-------------|--|--------|
| <b>1.269 Quinoline-2-carboxylic acid, 4-hydroxy- (Kynurenic acid)—Continued</b> |                                  |                        |                |                             |                             |                      |             |  |        |
|   | H <sub>2</sub> O<br>pH = 7.4     | air                    |                | 0.42                        |                             |                      | CP/Pa-43    | S' = RB; A = Im; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 332 nm. RNO as monitor of P.   | 91R141 |
| <b>1.270 Quinoxaline</b>  |                                  |                        |                |                             |                             |                      |             |  |        |
|   | C <sub>6</sub> H <sub>6</sub>    | air                    |                | ~0.91                       | ~0.91                       |                      | PL/Hp-52,42 | λ <sub>exc</sub> = 337 nm. Measured φ <sub>T</sub> ; assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, [S] > 5 × 10 <sup>-4</sup> mol L <sup>-1</sup> , Φ <sub>Δ</sub> = 0.73 extrapolating [S] → 0.  | 91F198 |
| <b>1.271 13-(Z)-Retinal</b>   |                                  |                        |                |                             |                             |                      |             |  |        |
|   | CCl <sub>4</sub>                 | air                    |                | 0.6                         |                             |                      | MP/LI-56    | S' = PPDME; rel. to Φ <sub>Δ</sub> (S') = 0.8; λ <sub>exc</sub> = 385 nm.  | 78F700 |
| <b>1.272 (all-E)-Retinal</b>  |                                  |                        |                |                             |                             |                      |             |  |        |
|   | c-C <sub>6</sub> H <sub>12</sub> | air                    |                | 1                           |                             |                      | PL/Ad-49,39 | A = DPBF; AC = S; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 5 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 3.4 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ε <sub>T</sub> (AC) not given.   | 85F041 |
|   | c-C <sub>6</sub> H <sub>12</sub> | O <sub>2</sub>         |                | 0.66 <sup>T</sup>           | ~1                          |                      | PL/Ad-49,42 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 5.0 × 10 <sup>4</sup> s <sup>-1</sup> , k <sub>A</sub> = 3.4 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , φ <sub>T</sub> (S) = 0.4–0.7 <sup>f</sup> , φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.   | 84F005 |
|   | CCl <sub>4</sub>                 | air                    |                | 0.6 <sup>T</sup>            |                             |                      | MP/LI-56    | S' = PPDME; rel. to Φ <sub>Δ</sub> (S') = 0.8; λ <sub>exc</sub> = 385 nm.  | 78F700 |
|   | EtOH                             | O <sub>2</sub>         |                | 0.096 <sup>T</sup>          |                             |                      | CP/Ac-15    | A = 2,5-DMF; λ <sub>exc</sub> = 365 nm.  | 78F201 |
|   | MeOH                             | air                    |                | 0.13 <sup>T</sup>           | 1                           |                      | PL/Ad-49,39 | A = DPBF; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 1 × 10 <sup>5</sup> s <sup>-1</sup> , k <sub>A</sub> = 8 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , φ <sub>T</sub> (S) = 0.12 <sup>c</sup> . ε <sub>T</sub> (AC) not given.  | 85F041 |
|   | MeOH                             | O <sub>2</sub>         |                | 0.20 <sup>T</sup>           | ~1                          |                      | PL/Ad-49,42 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used k <sub>d</sub> = 1.0 × 10 <sup>5</sup> s <sup>-1</sup> , k <sub>A</sub> = 8.1 × 10 <sup>8</sup> L mol <sup>-1</sup> s <sup>-1</sup> , φ <sub>T</sub> (S) = 0.12 <sup>f</sup> , φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7600 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm.  | 84F005 |
| <b>1.273 (all-E)-Retinol</b>  |                                  |                        |                |                             |                             |                      |             |  |        |
|   | n-C <sub>6</sub> H <sub>14</sub> | air                    |                | 0.78                        |                             |                      | PL/Ad-61    | S' = NMTA; A = DPBF; TD = NMTA; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 1.1; λ <sub>exc</sub> = 337 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for S quenching.  | 85E190 |
|   | n-C <sub>6</sub> H <sub>14</sub> | 1.4 × 10 <sup>-4</sup> |                | 0.25                        |                             |                      | PL/Ad-43    | S' = An; A = DPBF; TD = Triphenylene; rel. to Φ <sub>Δ</sub> (S') = 0.81; λ <sub>exc</sub> = 254 nm. Used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, f <sub>Δ</sub> <sup>T</sup> (S') = 1.   | 83E084 |
|   | C <sub>6</sub> H <sub>6</sub>    | var                    |                |                             | 0.42                        |                      | PL/Ad-49,39 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used ε <sub>T</sub> (AC) = 7.630 L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured f <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.36, f <sub>Δ</sub> <sup>S</sup> + (f <sub>Δ</sub> <sup>T</sup> - φ <sub>T</sub> )f <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.71, used f <sub>Δ</sub> <sup>T</sup> = 0.75. | 85E190 |
|   | C <sub>6</sub> H <sub>6</sub>    | air                    |                | 0.75                        |                             |                      | PL/Ad-61    | S' = NMTA; A = DPBF; TD = NMTA; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.92; λ <sub>exc</sub> = 337 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for S quenching.   | 85E190 |
|   | MeOH                             | var.                   |                |                             | 0.30                        |                      | PL/Ad-49,39 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; measured f <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.47, f <sub>Δ</sub> <sup>S</sup> + (f <sub>Δ</sub> <sup>T</sup> - φ <sub>T</sub> )f <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.68, used f <sub>Δ</sub> <sup>T</sup> = 0.72.  | 85E190 |
|   | MeOH                             | air                    |                | 0.78                        |                             |                      | PL/Ad-61    | S' = Ru(bpy) <sub>3</sub> <sup>2+</sup> ; A = DPBF; TD = Ru(bpy) <sub>3</sub> <sup>2+</sup> ; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.92; λ <sub>exc</sub> = 337 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for S quenching.   | 85E190 |
| <b>1.274 Riboflavin (RF)</b>  |                                  |                        |                |                             |                             |                      |             |  |        |
|   | D <sub>2</sub> O                 | air <sup>a</sup>       |                | 0.3                         |                             |                      | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8. Reference value in CCl <sub>4</sub> .  | 82Z317 |
|   | H <sub>2</sub> O<br>pH = 7.4     | air                    |                | 0.49                        |                             |                      | CP/Pa-43    | S' = RB; A = Im; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 445 nm. RNO as monitor of P.   | 91R141 |

Table 1, Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]            | Φ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method      | Comment  | Ref.   |
|---|---|------------------------------|-------------------|-----------------------------|-----------------------------|----------------------|-------------|--|--------|
| <b>1.274 Riboflavin (RF)—Continued</b>                              |   |                              |                   |                             |                             |                      |             |  |        |
|   | H <sub>2</sub> O/EtOH (1:1)                   | air <sup>a</sup>             | 0.5               |                             |                             |                      | PL/LI-56    | S' = RF; rel. to Φ <sub>Δ</sub> (S') = 0.3 <sup>b</sup> ; λ <sub>exc</sub> = 337 nm.<br>Rel. to RF in D <sub>2</sub> O.  | 86F144 |
|   | MeOD  | ~10 <sup>-3</sup>            | 0.58*             | 0.48                        | 0.79                        |                      | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; meas. Φ <sub>T</sub> (S) = 0.61; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in EtOH; recalcd. using Φ <sub>Δ</sub> (S') = 0.64 [88Z155].  | 88A165 |
|   | MeOH  | air <sup>a</sup>             | 0.47              |                             |                             |                      | PL/LI-56    | S' = Ery; rel. to Φ <sub>Δ</sub> (S') = 0.60.  | 87R138 |
|   | MeOH  | air <sup>a</sup>             | 0.4               |                             |                             |                      | PL/LI-56    | S' = RF; rel. to Φ <sub>Δ</sub> (S') = 0.3 <sup>b</sup> ; λ <sub>exc</sub> = 337 nm.<br>Rel. to RF in D <sub>2</sub> O.  | 86F144 |
| <b>1.275 Riboflavin 5'-dihydrogen phosphate (FMN)</b>               |   |                              |                   |                             |                             |                      |             |  |        |
|   | H <sub>2</sub> O pH = 7.4                     | air                          | 0.49              |                             |                             |                      | CP/Pa-43    | S' = RB; A = Im; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 445 nm. RNO as monitor of P.   | 91R141 |
| <b>1.276 Riboflavin-2',3',4',5'-tetraacetate</b>                    |   |                              |                   |                             |                             |                      |             |  |        |
|   | CH <sub>3</sub> CN                            | O <sub>2</sub>               | 0.65              |                             |                             |                      | CP/Pa-14    | λ <sub>exc</sub> = 442 nm. A = Oleic, linoleic or linolenic acid; hydroperoxide formation.   | 89F484 |
| <b>1.277 Rubicene (Benz(a)indeno(1,2,3-<i>hi</i>)aceanthrylene)</b> |   |                              |                   |                             |                             |                      |             |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          | 0.31              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          | 0.24              |                             |                             |                      | CP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.67.  | 88E609 |
|   | CCl <sub>4</sub>                              | air                          | 0.30              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
|   | CH <sub>3</sub> CN                            | air                          | 0.18              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
|   | CHCl <sub>3</sub>                             | air                          | 0.31              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
|   | CS <sub>2</sub>                               | air                          | 0.46              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
|   | ClCF <sub>2</sub> CCl <sub>2</sub> F          | air                          | 0.23              |                             |                             |                      | CP/Ac-14    | A = MDH. f <sub>T</sub> <sup>A</sup> = 0.30.   | 89E223 |
| <b>1.278 Rubrene (Tetracene, 5,6,11,12-tetraphenyl-, Rub)</b>       |   |                              |                   |                             |                             |                      |             |  |        |
|   | c-C <sub>6</sub> H <sub>12</sub>              | O <sub>2</sub>               | 0.95              |                             |                             | 1.4                  | CP/Ac-14,38 | S' = A = DPBF; λ <sub>exc</sub> = 546 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1;<br>Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.67 and Φ <sub>T</sub> = 0.   | 79E611 |
|   | n-C <sub>6</sub> H <sub>14</sub>              | O <sub>2</sub>               | 1.1               |                             |                             | 1.5                  | CP/Ac-14,38 | S' = A = DPBF; λ <sub>exc</sub> = 546 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1;<br>Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.78 and Φ <sub>T</sub> = 0.   | 79E611 |
|   | n-C <sub>6</sub> H <sub>14</sub>              | O <sub>2</sub>               | 1.2               | ≥0.54                       | ≥0.54                       |                      | CP/Ac-27    | A = 2,5-DMF; λ <sub>exc</sub> = 313 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1;<br>assumes f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used p <sub>A</sub> = 1.  | 79E643 |
|   | i-octane                                      | O <sub>2</sub>               | 1.1               |                             |                             | 1.4                  | CP/Ac-14,38 | S' = A = DPBF; λ <sub>exc</sub> = 546 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1;<br>Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.76 and Φ <sub>T</sub> = 0.   | 79E611 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air                          |                   |                             |                             | 2                    | PL/Ad,St-48 | A = S; λ <sub>exc</sub> = 530 nm; used k <sub>d</sub> = 3.2 × 10 <sup>4</sup> s <sup>-1</sup> ,<br>k <sub>A</sub> = 2.5 × 10 <sup>7</sup> L mol <sup>-1</sup> s <sup>-1</sup> , ε <sub>T</sub> (S) = 26000 L<br>mol <sup>-1</sup> cm <sup>-1</sup> at 500 nm. n <sub>Δ</sub> = 2.                            | 82E072 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | (0.6-1.2) × 10 <sup>-3</sup> |                   |                             |                             |                      | CP/Ac-14,38 | A = S; λ <sub>exc</sub> = 436 nm. Measured f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> f <sub>T</sub> <sup>O<sub>2</sub></sup><br>= 1.6  | 756223 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | O <sub>2</sub> (10 atm)      | 1.8               |                             |                             |                      | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.  | 82E010 |
|   | C <sub>6</sub> H <sub>6</sub>                 | (0.6-1.2) × 10 <sup>-3</sup> |                   |                             |                             |                      | CP/Ac-14,38 | A = S; λ <sub>exc</sub> = 436 nm. Measured f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> f <sub>T</sub> <sup>O<sub>2</sub></sup><br>= 1.7.   | 756223 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 1.8 × 10 <sup>-3</sup>       | 0.36              |                             |                             |                      | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50;<br>λ <sub>exc</sub> = 535, 546, 577 nm. rel. to S' in MeOH.  | 83F608 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 1.9 × 10 <sup>-3</sup>       | 0.30              |                             |                             |                      | CP/Ac-46    | S' = BP; A = S; rel. to Φ <sub>Δ</sub> (S') = 0.54; λ <sub>exc</sub> = 365 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 81F364 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          | 0.44              |                             |                             |                      | CP/Ac-14    | A = S; λ <sub>exc</sub> = 365 nm.  | 81F017 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>             | 0.07 <sup>T</sup> |                             |                             | 1.9                  | CP/Ac-14,40 | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> from Φ <sub>Δ</sub><br>when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 1; Φ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> = Φ <sub>Δ</sub> when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. | 767422 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>             |                   | ≥0.67                       | ≥1.7                        |                      | CP/Ac-14,38 | A = S. Assumed f <sub>Δ</sub> <sup>T</sup> = 1 and f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 76F905 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 4.6 × 10 <sup>-3</sup>       | 0.64              |                             |                             |                      | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50;<br>λ <sub>exc</sub> = 535, 546, 577 nm. rel. to S' in MeOH.  | 83F608 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]            | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method       | Comment  | Ref.   |
|---|---|------------------------------|-------------------|----------------|----------------|----------------------------|--------------|--|--------|
| <b>1.278 Rubrene (Tetracene, 5,6,11,12-tetraphenyl-, Rub)—Continued</b> |   |                              |                   |                |                |                            |              |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | 6.5 × 10 <sup>-3</sup>       | 1.0               |                |                |                            | CP/Pa-14     | A = S; P = 5,12-Dihydro-5,6,11,12-tetraphenyl-5,12-epidioxytetracene; $\lambda_{exc}$ = 546 nm.  | 337002 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub> var.          |                   |                |                |                            | CP/Ac-14,38  | A = S; $\lambda_{exc}$ = 435.8 nm. $\phi_T f_{\Delta}^T / (f_{\Delta}^T + f_{\Delta}^S) = 0.04 \pm 0.02$ .   | 68F286 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 9.1 × 10 <sup>-3</sup>       | 0.90              |                |                |                            | CP/Oc-43     | S' = MB <sup>+</sup> ; A = TME; rel. to $\phi_A(S') = 0.50$ ; $\lambda_{exc}$ = 535, 546, 577 nm. rel. to S' in MeOH; $\phi_T f_{\Delta}^T = 0.03 (P_S^{O_2} = 0); f_{\Delta}^S + f_{\Delta}^T f_T^{O_2} = 1.5$  | 83F608 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 9.0 × 10 <sup>-3</sup>       | 0.88              |                |                | 1.4                        | CP/Ac-46     | S' = BP; A = S; rel. to $\phi_A(S') = 0.90$ ; $\lambda_{exc}$ = 365 nm; used $P_T(S) = 0.03$ . Assumed $f_T^{O_2} = 1$ .   | 81F364 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.91              |                |                | 1.5                        | CP/Ac-14,38  | S' = A = DPBF; $\lambda_{exc}$ = 546 nm. $P_T^{O_2} = 1$ ; Assumed $f_T^{O_2} = 1$ ; used $P_S^{O_2} = 0.62$ and $\phi_T = 0$ .  | 79E611 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 1 <sup>ST</sup>   |                |                |                            | CP/Ac-14     | A = S; $\lambda_{exc}$ = 366, 436, 546 nm.   | 34F004 |
|   | C <sub>6</sub> H <sub>6</sub>                 | → ∞                          | 1.2 <sup>ST</sup> |                |                | ~1.2                       | CP/Ac-14,38  | A = DPBF; $\lambda_{exc}$ = 545 nm. Assumed $f_T^{O_2} = 1$ , extrapolated $\phi_{\Delta} = 1.2$ when [O <sub>2</sub> ] → ∞.   | 78E036 |
|   | CH <sub>3</sub> COCH <sub>3</sub>             | O <sub>2</sub>               | 0.88              |                |                | 1.5                        | CP/Ac-14,38  | S' = A = DPBF; $\lambda_{exc}$ = 546 nm. $P_T^{O_2} = 1$ ; Assumed $f_T^{O_2} = 1$ ; used $P_S^{O_2} = 0.58$ and $\phi_T = 0$ .  | 79E611 |
|   | CHCl <sub>3</sub>                             | (0.3-5) × 10 <sup>-3</sup>   |                   |                |                |                            | CP/Ac-14,38  | A = S; $\lambda_{exc}$ = 436 nm. Assumed $f_T^{O_2} = 1, f_{\Delta}^T = f_{\Delta}^S = 1$ , measured $f_{\Delta}^T + f_{\Delta}^S f_T^{O_2} = 2.1$ ; $\phi_{\Delta} = 0.11$ when $P_S^{O_2} = 0$ .   | 756223 |
|   | C <sub>6</sub> H <sub>5</sub> Cl <sub>3</sub> | (0.5-2.5) × 10 <sup>-3</sup> |                   |                |                |                            | CP/Ac-14,38  | A = S; $\lambda_{exc}$ = 436 nm. Measured $f_{\Delta}^T + f_{\Delta}^S f_T^{O_2} = 1.7$ .  | 756223 |
|   | CCl <sub>4</sub>                              | (0.3-3) × 10 <sup>-3</sup>   |                   |                |                |                            | CP/Ac-14,38  | A = S; $\lambda_{exc}$ = 436 nm. Measured $f_{\Delta}^T + f_{\Delta}^S f_T^{O_2} = 1.9$ .  | 756223 |
|   | CS <sub>2</sub>                               | (0.5-1) × 10 <sup>-3</sup>   |                   |                |                |                            | CP/Ac-14,38  | A = S; $\lambda_{exc}$ = 436 nm. Measured $f_{\Delta}^T + f_{\Delta}^S f_T^{O_2} = 2.1$  | 756223 |
|   | CS <sub>2</sub>                               | (2-9) × 10 <sup>-3</sup>     |                   | 1              | 1              | 2                          | CP/Ac-14,38  | A = DPBF; $\lambda_{exc}$ = 546 nm. Assumed $f_T^{O_2} = 1$ , $\phi_T f_{\Delta}^T = 0.21$ .   | 84F197 |
| <b>1.279 (E)-Stilbene</b>   |   |                              |                   |                |                |                            |              |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>             |                   | ~0.08          |                |                            | PR/βCb-59    | S' = BP; rel. to $f_{\Delta}^T(S') = 0.35$ . Measured $f_{\Delta}^T(S) / f_{\Delta}^T(S') = 0.23$ .  | 76F904 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               |                   | 0.21*          |                |                            | PL/LI-60     | S' = 2-ACN; rel. to $f_{\Delta}^T(S') = 0.7$ ; $\lambda_{exc}$ = 355 nm. $P_T^{O_2} > 0.96$ .  | 85F291 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               |                   | 0.18           |                |                            | PL/LI-60     | S' = BP; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc}$ = 355 nm. $P_T^{O_2} > 0.96$ .  | 85F291 |
| <b>1.280 Sydnone, 3,4-diphenyl-</b>                                     |   |                              |                   |                |                |                            |              |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          |                   | 0.78           |                |                            | PL/Ad,TDt-62 | A = DPBF; AC = TD = NMTA; $\lambda_{exc}$ = 485 nm; used $k_d = 4.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 8.0 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(AC) = 9300 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. $P_T^{O_2} = 0.82$ . | 86A380 |
| <b>1.281 Sydnone, 3-(4-methylphenyl)-</b>                               |   |                              |                   |                |                |                            |              |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          |                   | 0.38           |                |                            | PL/Ad,TDt-62 | A = DPBF; AC = TD = CQ; $\lambda_{exc}$ = 485 nm; used $k_d = 4.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 8.0 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(AC) = 900 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 700 nm. $P_T^{O_2} = 0.89$ .    | 86A380 |
| <b>1.282 Sydnone, 3-(4-methylphenyl)-4-phenyl-</b>                      |   |                              |                   |                |                |                            |              |  |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          |                   | 0.88           |                |                            | PL/Ad,TDt-62 | A = DPBF; AC = TD = NMTA; $\lambda_{exc}$ = 485 nm; used $k_d = 4.0 \times 10^4 \text{ s}^{-1}$ , $k_A = 8.0 \times 10^8 \text{ L mol}^{-1} \text{ s}^{-1}$ , $\epsilon_T(AC) = 9300 \text{ L mol}^{-1} \text{ cm}^{-1}$ at 520 nm. $P_T^{O_2} = 0.78$ . | 86A380 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                  | [O <sub>2</sub> ]          | $\phi_{\Delta}$   | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method         | Comment  | Ref.   |
|-------|--|----------------------------|-------------------|----------------|----------------|----------------------------|----------------|--|--------|
| 1.283 | Sydnone, 3-phenyl-                       |                            |                   |                |                |                            |                |  |        |
|       | C <sub>6</sub> H <sub>6</sub>            | air                        |                   | 0.80           |                |                            | PL/Ad,TDt-62   | A = DPBF; AC = TD = CQ; $\lambda_{exc} = 485$ nm; used $k_d = 4.0 \times 10^4$ s <sup>-1</sup> , $k_A = 8.0 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> , $\epsilon_T(AC) = 900$ L mol <sup>-1</sup> cm <sup>-1</sup> at 700 nm. $P_T^{O_2} = 0.88$ . | 86A380 |
| 1.284 | p-Terphenyl                              |                            |                   |                |                |                            |                |  |        |
|       | C <sub>6</sub> H <sub>6</sub>            | O <sub>2</sub>             |                   | 0.9            |                |                            | PR/Ad,St-49,42 | A = DPBF; used $\phi_T(S) = 0.11$ , $\epsilon_T(S) = 90,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm. Measured $G(^3S^*)$ .   | 78E263 |
| 1.285 | $\alpha$ -Terthienyl                     |                            |                   |                |                |                            |                |  |        |
|       | C <sub>6</sub> D <sub>6</sub>            | (1.9-9.1) $\times 10^{-3}$ | 0.67 <sup>T</sup> |                |                |                            | PL/LI-56       | S' = Np; rel. to $\phi_{\Delta}(S') = 0.54$ ; $\lambda_{exc} = 355$ nm.  | 90E691 |
|       | C <sub>6</sub> D <sub>6</sub>            | (1.9-9.1) $\times 10^{-3}$ | 0.84 <sup>T</sup> |                |                |                            | PL/LI-56       | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 90E691 |
|       | C <sub>6</sub> H <sub>6</sub>            | air                        | 0.75 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | CD <sub>3</sub> CN                       | (1.7-8.1) $\times 10^{-3}$ | 0.79 <sup>T</sup> |                |                |                            | PL/LI-56       | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 90E691 |
|       | CD <sub>3</sub> OD                       | air                        | 0.67 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = An; rel. to $\phi_{\Delta}(S') = 0.55$ ; meas. $\phi_T(S) = -0.9-1.0$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | CD <sub>3</sub> OD                       | air                        | 0.70 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Ru(bpy) <sub>3</sub> <sup>2+</sup> ; rel. to $\phi_{\Delta}(S') = 0.86$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.  | 90F355 |
|       | CDCl <sub>3</sub>                        | air                        | 0.73 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.84$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | CDCl <sub>3</sub>                        | $\sim 1.16 \times 10^{-2}$ | 0.86 <sup>T</sup> |                |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. $p_A = 1$ .   | 87E410 |
|       | CH <sub>2</sub> Cl <sub>2</sub>          | air                        | 0.75 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.89$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | CH <sub>3</sub> CN                       | air                        | 0.68 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.82$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | CHCl <sub>3</sub>                        | air                        | 0.67 <sup>T</sup> | ~0.7           |                |                            | PL/LI-56,42    | S' = Pz; rel. to $\phi_{\Delta}(S') = 0.84$ ; meas. $\phi_T(S) = -0.9-1$ ; $\lambda_{exc} = 337$ nm.   | 90F355 |
|       | EtOH                                     | O <sub>2</sub>             | $\sim 0.2^T$      | ~1             |                |                            | PL/Ac-14,42    | A = DPBF; meas. $\phi_T(S) = 0.20^f$ ; $\lambda_{exc} = 353$ nm. $P_T^{O_2} = 1$ , $p_A = 0.75$ .  | 85N020 |
|       | EtOH/H <sub>2</sub> O<br>(95:5)          | air                        | 0.22 <sup>T</sup> | ~1             |                |                            | CP/Ac-14,42    | A = Im; $\lambda_{exc} = 365$ nm; used $\phi_T(S) = 0.20$ .  | 89F115 |
| 1.286 | 2,2':5',2''-Terthiophene, 5-bromo-       |                            |                   |                |                |                            |                |  |        |
|       | CDCl <sub>3</sub>                        | $\sim 1.16 \times 10^{-2}$ | 0.70 <sup>T</sup> |                |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. $p_A = 1$ .   | 87E410 |
| 1.287 | 2,2':5',2''-Terthiophene, 5-cyano-       |                            |                   |                |                |                            |                |  |        |
|       | CDCl <sub>3</sub>                        | $\sim 1.16 \times 10^{-2}$ | 0.86 <sup>T</sup> |                |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. $p_A = 1$ .   | 87E410 |
| 1.288 | 2,2':5',2''-Terthiophene, 5,5''-dibromo- |                            |                   |                |                |                            |                |  |        |
|       | CDCl <sub>3</sub>                        | $\sim 1.16 \times 10^{-2}$ | 0.69 <sup>T</sup> |                |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. $p_A = 1$ .   | 87E410 |
|       | EtOH                                     | O <sub>2</sub>             | $\sim 0.3^T$      | ~1             |                |                            | PL/Ac-14,42    | A = DPBF; meas. $\phi_T(S) = 0.35^f$ ; $\lambda_{exc} = 353$ nm. $P_T^{O_2} = 1$ , $p_A = 0.75$ .  | 85N020 |
| 1.289 | 2,2':5',2''-Terthiophene, 5-methyl-      |                            |                   |                |                |                            |                |  |        |
|       | CDCl <sub>3</sub>                        | $\sim 1.16 \times 10^{-2}$ | 0.93 <sup>T</sup> |                |                |                            | PL/Ad,ACt-49   | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $\phi_T(AC) = 1$ , $\epsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. $p_A = 1$ .   | 87E410 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]            | Φ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | f <sub>Δ</sub> <sup>S</sup> | Σf or n <sub>Δ</sub> | Method       | Comment   | Ref.             |
|---|---|------------------------------|-------------------|-----------------------------|-----------------------------|----------------------|--------------|---|------------------|
| <b>1.290 2,2':5',2''-Terthiophene-5-carboxylic acid</b> |   |                              |                   |                             |                             |                      |              |   |                  |
|   | EtOH  | O <sub>2</sub>               | ~0.2 <sup>T</sup> | ~1                          |                             |                      | PL/Ac-14,42  | A = DPBF; meas. Φ <sub>T</sub> (S) = 0.2 <sup>f</sup> , λ <sub>exc</sub> = 353 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, p <sub>A</sub> = 0.75.  | 85N020           |
| <b>1.291 Tetracene</b>                                  |   |                              |                   |                             |                             |                      |              |   |                  |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | O <sub>2</sub>               | 0.86              |                             |                             |                      | PL/LI-38,56  | used Φ <sub>T</sub> (S) = 0.61. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> = 1.2.  | 87E668           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 0.2 atm O <sub>2</sub>       | 0.71              |                             |                             |                      | PL/LI-38,56  | used Φ <sub>T</sub> (S) = 0.61. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> = 1.2.  | 87E668           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | (2-9) × 10 <sup>-3</sup>     |                   |                             |                             | 1.2                  | CP/Ac-14,38  | A = DPBF; λ <sub>exc</sub> = 470 nm. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, Φ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> = 0.61.  | 84F197           |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          | 0.70              |                             |                             |                      | CP/Ac-40     | A = DPBF. Assumed f <sub>Δ</sub> <sup>S</sup> = 0, f <sub>Δ</sub> <sup>T</sup> = 1.   | 78E036           |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.83              |                             |                             |                      | CP/Ac-40     | A = DPBF. Assumed f <sub>Δ</sub> <sup>S</sup> = 0, f <sub>Δ</sub> <sup>T</sup> = 1.   | 78E036           |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                          | 0.68              |                             |                             |                      | CP/Ac-14     | A = DPBF.   | 78E036           |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.85              |                             |                             |                      | CP/Ac-14     | A = DPBF.   | 78E036           |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>             | 0.71 <sup>T</sup> |                             |                             | 1.2                  | CP/Ac-14,40  | A = S. Assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> from Φ <sub>Δ</sub> when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 1; Φ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> = Φ <sub>Δ</sub> when P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. | 767422           |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>             |                   | ~1                          | ~0                          | ~1                   | CP/Ac-14,38  | A = S. Assumed f <sub>Δ</sub> <sup>T</sup> = 1 and f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 76F905           |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub> var.          |                   |                             |                             |                      | CP/Ac-14,38  | A = S; λ <sub>exc</sub> = 435.8 nm. Φ <sub>T</sub> f <sub>Δ</sub> <sup>T</sup> / (f <sub>Δ</sub> <sup>T</sup> + f <sub>Δ</sub> <sup>S</sup> ) = 0.61.   | 68F286           |
| <b>1.292 α-Tetralone</b>                                |   |                              |                   |                             |                             |                      |              |   |                  |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.25 <sup>T</sup> | 0.25                        |                             |                      | PL/Hp-52,42  | λ <sub>exc</sub> = 355 nm; used Φ <sub>T</sub> (S) = 1. Measured Φ <sub>Δ</sub> = 0.25, P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 and Φ <sub>F</sub> .  | 88E449           |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.29 <sup>T</sup> | 0.25                        |                             |                      | PL/LI-56,42  | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83; used Φ <sub>T</sub> (S) = 1. Measured P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 88E449           |
| <b>1.293 Thiobenzophenone, 4,4'-dimethoxy- (DMTBP)</b>  |   |                              |                   |                             |                             |                      |              |   |                  |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>               | 0.88*             | 1.0 <sup>T</sup>            | 1.0                         |                      | PL/Ad-43,42  | S' = BP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.4; meas. Φ <sub>T</sub> (S) = 1 <sup>f</sup> ; λ <sub>exc</sub> = 337 nm. Assumed Φ <sub>T</sub> (S) = Φ <sub>T</sub> (S').  | 84A221           |
|   | CHCl <sub>3</sub>                             | air <sup>a</sup>             | 1.0 <sup>T</sup>  | 1.0                         |                             |                      | CP/Ac-14,42  | A = DTBF; used Φ <sub>T</sub> (S) = 1. [S] → 0, Φ <sub>Δ</sub> = 0.83 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| <b>1.294 Thiobenzophenone, 4-phenyl-</b>                |   |                              |                   |                             |                             |                      |              |   |                  |
|   | CHCl <sub>3</sub>                             | air <sup>a</sup>             | 1.0 <sup>T</sup>  | 1.0                         |                             |                      | CP/Ac-14,42  | A = DTBF; used Φ <sub>T</sub> (S) = 1. [S] → 0, Φ <sub>Δ</sub> = 0.56 at [S] = 0.01 mol L <sup>-1</sup> .   | 83F028<br>82F140 |
| <b>1.295 Thiocoumarin</b>                               |   |                              |                   |                             |                             |                      |              |   |                  |
|   | C <sub>6</sub> H <sub>6</sub>                 | (1.9-9.1) × 10 <sup>-3</sup> | 0.7*              | 0.8 <sup>T</sup>            | 0.8                         |                      | PL/Ad-43,39  | S' = BP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.4; meas. Φ <sub>T</sub> (S) = 1; λ <sub>exc</sub> = 337 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.  | 86A240           |
|   | C <sub>6</sub> H <sub>6</sub>                 | (1.9-9.1) × 10 <sup>-3</sup> | 1.0 <sup>T</sup>  | 1.0                         |                             |                      | PL/Ad-43,39  | S' = DMTBP; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 1; meas. Φ <sub>T</sub> (S) = 1; λ <sub>exc</sub> = 532 nm. Used P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 86A240           |
| <b>1.296 Thiophene, 2,5-diphenyl-</b>                   |   |                              |                   |                             |                             |                      |              |   |                  |
|   | EtOH  | O <sub>2</sub>               | ~0.3              | ~1                          |                             |                      | PL/Ac-14,42  | A = DPBF; meas. Φ <sub>T</sub> (S) = 0.30; λ <sub>exc</sub> = 353 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, p <sub>A</sub> = 0.75.   | 85N020           |
| <b>1.297 Thiophene, 2-(1-naphthalenyl)-</b>             |   |                              |                   |                             |                             |                      |              |   |                  |
|   | CDCl <sub>3</sub>                             | ~1.16 × 10 <sup>-2</sup>     | 0.76 <sup>T</sup> |                             |                             |                      | PL/Ad,ACt-49 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 525 L mol <sup>-1</sup> cm <sup>-1</sup> at 7640 nm. p <sub>A</sub> = 1.  | 87E410           |
| <b>1.298 Thiophene, 2-(2-naphthalenyl)-</b>             |   |                              |                   |                             |                             |                      |              |   |                  |
|   | CDCl <sub>3</sub>                             | ~1.16 × 10 <sup>-2</sup>     | 0.63 <sup>T</sup> |                             |                             |                      | PL/Ad,ACt-49 | A = DPBF; AC = BP; λ <sub>exc</sub> = 337 nm; used Φ <sub>T</sub> (AC) = 1, ε <sub>T</sub> (AC) = 7640 L mol <sup>-1</sup> cm <sup>-1</sup> at 525 nm. p <sub>A</sub> = 1.  | 87E410           |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]                  | $\phi_{\Delta}$    | $f_{\Delta}^T$    | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method       | Comment  | Ref.   |
|-------|---|------------------------------------|--------------------|-------------------|----------------|----------------------------|--------------|--|--------|
| 1.299 | Thiophene, 2,2'-(1,3-phenylene)bis-<br>CDCl <sub>3</sub>                              | $\sim 1.16 \times 10^{-2}$         | 0.75 <sup>T</sup>  |                   |                |                            | PL/Ad,ACt-49 | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used<br>$\phi_T(AC) = 1$ , $\varepsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at<br>525 nm. $p_A = 1$ .  | 87E410 |
| 1.300 | Thiophene, 2,2'-(1,4-phenylene)bis-<br>CDCl <sub>3</sub>                              | $\sim 1.16 \times 10^{-2}$         | 0.69 <sup>T</sup>  |                   |                |                            | PL/Ad,ACt-49 | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used<br>$\phi_T(AC) = 1$ , $\varepsilon_T(AC) = 7640$ L mol <sup>-1</sup> cm <sup>-1</sup> at<br>525 nm. $p_A = 1$ .  | 87E410 |
| 1.301 | 4-Thiouridine   |                                    |                    |                   |                |                            |              |  |        |
|       | CH <sub>3</sub> CN  | air                                | 0.6 <sup>T</sup>   | 1                 |                |                            | PL/LI-56,42  | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.84$ ; meas. $\phi_T(S) = 0.61$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 0.92$ .  | 90E312 |
|       | CH <sub>3</sub> CN  | O <sub>2</sub>                     | 0.4 <sup>T</sup>   | 0.67              |                |                            | PL/Hp-53,42  | meas. $\phi_T(S) = 0.61$ ; $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 0$ . $P_T^{O_2} = >0.98$ .  | 90E312 |
|       | CH <sub>3</sub> CN  | O <sub>2</sub>                     | 0.5 <sup>T</sup>   | 0.84              |                |                            | PL/Hp-52,42  | meas. $\phi_T(S) = 0.61$ ; $\lambda_{exc} = 353$ nm. $P_T^{O_2} = >0.98$ .   | 90E312 |
|       | CH <sub>3</sub> CN  | O <sub>2</sub>                     | 0.70 <sup>T</sup>  |                   |                |                            | PL/LI-56,42  | S' = DCA; rel. to $\phi_{\Delta}(S') = 1.6$ ; $\lambda_{exc} = 355$ nm.  | 83F604 |
|       | D <sub>2</sub> O  | air                                | 0.18 <sup>T</sup>  | 0.93              |                |                            | PL/LI-56,42  | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to $\phi_{\Delta}(S') = 0.80$ ; meas. $\phi_T(S) = 0.67$ ; $\lambda_{exc} = 353$ nm. $P_T^{O_2} = 0.29$ .   | 90E312 |
| 1.302 | 1,4,7-Triazacyclononanetri(isothiocyanato)chromium(III) (Cr(tacn)(NCS) <sub>3</sub> ) | (CH <sub>3</sub> ) <sub>2</sub> CO | O <sub>2</sub>     | 0.62              |                |                            | CP/Pa-43     | S' = RB; A = Furan; P = Furan endoperoxide;<br>rel. to $\phi_{\Delta}(S') = 0.80^b$ .  | 89F067 |
| 1.303 | Tribenzo[a,f,j]perylene, 9,18-diphenyl- (Mesodiphenylbenzheianthrene, MDBH)           |                                    |                    |                   |                |                            |              |  |        |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH                                      | air                                | 0.17               |                   |                |                            | CP/Ac-A.18   | A = S; $\lambda_{exc} = 632.8$ nm. $f_r^A = 0.026$ .   | 87F480 |
|       | m-Cresol  | air                                | 0.12               |                   |                |                            | CP/Ac-A.18   | A = S; $\lambda_{exc} = 632.8$ nm; used $\phi_T(S) = 0.61$ .<br>$f_r^A = 0.026$ .  | 87F480 |
|       | CCl <sub>4</sub>  | air                                | 0.18               |                   |                |                            | CP/Ac-14,38  | A = S; meas. $\phi_T(S) = 0.09$ ; $\lambda_{exc} = 632.8$ nm.<br>$f_r^O_2 = 1$ , $f_r^A = 0.026$ , [O <sub>2</sub> ] varied, ( $f_{\Delta}^S + f_{\Delta}^T f_r^O_2$ ) = 0.91.   | 87F479 |
| 1.304 | Triphenylene  |                                    |                    |                   |                |                            |              |  |        |
|       | c-C <sub>6</sub> H <sub>12</sub>  | $\rightarrow \infty$               | 0.49 <sup>ST</sup> |                   |                |                            | PL/LI-56     | S' = Py; rel. to $\phi_{\Delta}(S') = 0.81$ ; $\lambda_{exc} = 355$ nm.  | 91E297 |
|       | n-C <sub>6</sub> H <sub>14</sub>  | air                                | 0.25               |                   |                |                            | PL/Ad-43     | S' = An; A = DPBF; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 264$ nm. $P_T^{O_2} = 1$ .   | 82E258 |
|       | CH <sub>3</sub> CN  | $\rightarrow \infty$               | 0.27 <sup>ST</sup> |                   |                |                            | PL/LI-56     | S' = DCA; rel. to $\phi_{\Delta}(S') = 2.0$ ; $\lambda_{exc} = 355$ nm.  | 91E297 |
| 1.305 | Tris(2,2'-bipyridine)iridium(III) ion   | MeOH                               | O <sub>2</sub>     | $\sim 1^T$        |                |                            | CL/Oc-14     | A = TME; $\lambda_{exc} = 488$ nm.   | 777221 |
| 1.306 | Tris(2,2'-bipyridine)ruthenium(II) ion  |                                    |                    |                   |                |                            |              |  |        |
|       | MeOH  | air <sup>a</sup>                   |                    | 0.81 <sup>T</sup> | 0.92           |                            | PL/Ad-49,39  | A = DPBF; AC = BP; $\lambda_{exc} = 532$ nm; used $k_d = 1.0 \times 10^5$ s <sup>-1</sup> , $k_A = 8.1 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> ,<br>$\phi_T(S) = 0.95^c$ , $\phi_T(AC) = 1$ , $\varepsilon_T(AC) = 7600$ L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. $P_T^{O_2} = 0.93$ . | 85E190 |
|       | MeOH  | O <sub>2</sub>                     |                    | 0.83 <sup>T</sup> | 0.94           |                            | PL/Ad-49,41  | A = DPBF; AC = BP; $\lambda_{exc} = 337$ nm; used $k_d = 1.0 \times 10^5$ s <sup>-1</sup> , $k_A = 8.1 \times 10^8$ L mol <sup>-1</sup> s <sup>-1</sup> ,<br>$\phi_T(S) = 0.95^d$ , $\phi_T(AC) = 1$ , $\varepsilon_T(AC) = 7600$ L mol <sup>-1</sup> cm <sup>-1</sup> at 532 nm. $P_T^{O_2} = 0.93$ . | 84F005 |
|       | MeOH  | O <sub>2</sub>                     |                    | 0.90 <sup>T</sup> | 0.95           |                            | CP/Ac-43,42  | S' = RB; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.80^b$ , $\lambda_{exc} = 546$ nm; used $\phi_T(S) = 0.95^d$ . Measured $P_T^{O_2} = 1$ .  | 80F304 |
|       | MeOH  | O <sub>2</sub>                     |                    | 0.86 <sup>T</sup> | 0.91           |                            | CL/Oc-14,42  | A = TME; $\lambda_{exc} = 488, 514.4, 457.9$ nm; used $\phi_T(S) = 0.95^d$ . Used $P_T^{O_2} = 1$ .  | 767423 |

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No.   | Solvent  | [O <sub>2</sub> ] | $\phi_{\Delta}$ | $f_{\Delta}^T$       | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method       | Comment   | Ref.   |
|-------|--|-------------------|-----------------|----------------------|----------------|----------------------------|--------------|---|--------|
| 1.307 | Tris(1,10-phenanthroline)iridium(III) ion  |                   |                 |                      |                |                            |              |   |        |
|       | MeOH   | O <sub>2</sub>    |                 | ~1 <sup>T</sup>      |                |                            | CL/Oc-14     | A = TME; $\lambda_{exc} = 488$ nm.  | 777221 |
| 1.308 | Tris(1,10-phenanthroline)osmium(II) ion  |                   |                 |                      |                |                            |              |   |        |
|       | MeOH   | O <sub>2</sub>    |                 | 0.76 <sup>T</sup>    |                |                            | CL/Oc-14     | A = TME; $\lambda_{exc} = 488$ nm.  | 777221 |
| 1.309 | Tris(1,10-phenanthroline)ruthenium(II) ion                                       |                   |                 |                      |                |                            |              |   |        |
|       | MeOH   | O <sub>2</sub>    |                 | 0.75 <sup>T</sup>    |                |                            | CL/Oc-14     | A = TME; $\lambda_{exc} = 488$ nm.  | 777221 |
|       | MeOH   | O <sub>2</sub>    |                 | 0.95 <sup>T</sup>    |                |                            | CL/Oc-14     | A = H <sub>2</sub> NCSNH <sub>2</sub> ; $\lambda_{exc} = 488$ nm.   | 777221 |
| 1.310 | Vitamin D <sub>3</sub>   |                   |                 |                      |                |                            |              |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  |                   |                 | 2 × 10 <sup>-3</sup> |                |                            |              |   |        |
|       |  |                   |                 |                      | 0.28*          |                            | PL/LI-60     |   |        |
|       |  |                   |                 |                      | 0.25           |                            |              | $S' = Np$ ; TD = p-MAP; rel. to $f_{\Delta}^T(S') = 0.55$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} \rightarrow 1$ ; Cor. for 12% oxygen quenching of p-MAP triplet. | 90E030 |
|       |  |                   |                 |                      |                |                            |              |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  |                   |                 | 2 × 10 <sup>-3</sup> |                |                            | PL/LI-60     | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.29$ ; $\lambda_{exc} = 355$ nm. Measured $P_T^{O_2}$ .  | 89A235 |
|       |  |                   |                 |                      | 0.30*          |                            |              |   |        |
|       |  |                   |                 |                      | 0.25           |                            |              |   |        |
| 1.311 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-4,5-diodo-, dianion                  |                   |                 |                      |                |                            |              |   |        |
|       | DMF  | air <sup>a</sup>  |                 | 0.30                 |                |                            | CP/Ac-43     | $S' = RB$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 88F618 |
| 1.312 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetrabromo-, dianion         |                   |                 |                      |                |                            |              |   |        |
|       | DMF  | air <sup>a</sup>  |                 | 0.13                 |                |                            | CP/Ac-43     | $S' = RB$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 88F618 |
| 1.313 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetraiodo-, dianion          |                   |                 |                      |                |                            |              |   |        |
|       | DMF  | air <sup>a</sup>  |                 | 0.44                 |                |                            | CP/Ac-43     | $S' = RB$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 88F618 |
| 1.314 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5-triiodo-, dianion              |                   |                 |                      |                |                            |              |   |        |
|       | DMF  | air <sup>a</sup>  |                 | 0.41                 |                |                            | CP/Ac-43     | $S' = RB$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 88F618 |
| 1.315 | Xanthen-3-one, 9-(2,3,4,5-tetrachlorophenyl)-6-hydroxy-2,4,5,7-tetraiodo-, anion |                   |                 |                      |                |                            |              |   |        |
|       | MeOH   | air <sup>a</sup>  |                 | 0.87                 |                |                            | CP/Ac-43     | $S' = Eos$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.32$ . Rel. to S' in ethanol.  | 90F251 |
|       | MeOH   | air <sup>a</sup>  |                 | 0.76                 |                |                            | CP/Ac-43     | $S' = RB$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 90F251 |
| 1.316 | Xanthen-9-one  |                   |                 |                      |                |                            |              |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>  |                 | 0.33 <sup>T</sup>    | 0.33           |                            | PL/βCb-43,42 | $S' = BP$ ; rel. to $f_{\Delta}^T(S') = 0.35$ ; used $\phi_T(S) = 1^d$ . Measured $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.95$ .                                   | 76F904 |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>    |                 | 0.24 <sup>T</sup>    | 0.28           |                            | PL/LI-56,42  | $S' = Pz$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; used $\phi_T(S) = 1$ . Measured $P_T^{O_2} = 0.82$ .   | 88E449 |
|       | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>    |                 | 0.28 <sup>T</sup>    | 0.28           |                            | PL/Hp-52,42  | $\lambda_{exc} = 355$ nm; used $\phi_T(S) = 1$ . Measured $\phi_{\Delta} = 0.23$ , $P_T^{O_2} = 0.82$ and $\phi_F$ .  | 88E449 |
| 1.317 | O <sub>2</sub> :solvent CT state   |                   |                 |                      |                |                            |              |   |        |
|       | Decalin  | air               |                 | ~0.12                |                |                            | PL/LI-56     | $S' = Biph$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 239$ nm.   | 89E309 |
|       | c-C <sub>6</sub> H <sub>12</sub>   | air               |                 | ~0.22                |                |                            | PL/LI-56     | $S' = Biph$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 239$ nm.   | 89E309 |
|       | c-C <sub>8</sub> H <sub>16</sub>   | air               |                 | ~0.18                |                |                            | PL/LI-56     | $S' = Biph$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 239$ nm.   | 89E309 |
|       | 1,3,5-C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>              | air               |                 | ~0.17                |                |                            | PL/LI-56     | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.8$ ; $\lambda_{exc} = 355$ nm.   | 89E309 |
|       | 1,2-C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>                | air               |                 | ~0.20                |                |                            | PL/LI-56     | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.8$ ; $\lambda_{exc} = 355$ nm.   | 89E309 |
|       | 1,4-C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>                | air               |                 | ~0.20                |                |                            | PL/LI-56     | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.8$ ; $\lambda_{exc} = 355$ nm.   | 89E309 |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | O <sub>2</sub>    |                 | 0.25                 |                |                            | PL/LI-56     | $S' = TPP$ ; rel. to $\phi_{\Delta}(S') = 0.82$ ; $\lambda_{exc} = 347$ nm.   | 90E760 |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                    | air               |                 | ~0.20                |                |                            | PL/LI-56     | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.8$ ; $\lambda_{exc} = 355$ nm.   | 89E309 |
|       | C <sub>6</sub> H <sub>6</sub>  | air               |                 | ~0.20                |                |                            | PL/LI-56     | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.8$ ; $\lambda_{exc} = 355$ nm.   | 89E309 |

<sup>a</sup> Oxygen concentration not given; assumed to be air saturated.<sup>b</sup> Value of  $\phi_{\Delta}(S')$  used in this work to calculate  $\phi_{\Delta}(S)$  from authors' reported  $\phi_{\Delta}(S)/\phi_{\Delta}(S')$ .

Table 1. Quantum yields of photosensitized production of singlet oxygen.—Continued

| No. | Solvent | [O <sub>2</sub> ] | $\phi_{\Delta}$ | $f_{\Delta}^T$ | $f_{\Delta}^S$ | $\Sigma f$ or $n_{\Delta}$ | Method | Comment | Ref. |
|-----|---------|-------------------|-----------------|----------------|----------------|----------------------------|--------|---------|------|
|-----|---------|-------------------|-----------------|----------------|----------------|----------------------------|--------|---------|------|

<sup>c</sup> Value of  $\phi_T(S)$  from the literature used in this work to calculate  $\phi_{\Delta}$ .<sup>d</sup> Value of  $\phi_T(S)$  from the literature used in this work to calculate  $f_{\Delta}^T$ .<sup>e</sup> Value of  $\phi_T(S)$  measured or quoted by the authors, used in this work to calculate  $\phi_{\Delta}$ .<sup>f</sup> Value of  $\phi_T(S)$  measured or quoted by the authors, used in this work to calculate  $f_{\Delta}^T$ .<sup>g</sup> Value of  $\phi_T(S)$  used in this work to calculate  $\phi_{\Delta}$  or  $f_{\Delta}^T$ , average of 0.73 [776258] and 1.0 [81E147].<sup>T</sup> Value corrected for 100% quenching of T<sub>1</sub>.<sup>ST</sup> Value corrected for 100% quenching of S<sub>1</sub> and T<sub>1</sub>.\* Values recalculated using  $\phi_{\Delta}(S')$  or  $f_{\Delta}^T(S')$  from Table 4 or from the quoted reference.

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.

| No.                                     | Solvent  | [O <sub>2</sub> ]                     | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment  | Ref.             |
|---|--|---------------------------------------|----------------|-----------------------------|-------------|--|------------------|
| <b>2.1 Bacteriochlorophyll <i>a</i></b> |  |                                       |                |                             |             |  |                  |
|   | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup>                      | 0.43           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | C <sub>5</sub> H <sub>5</sub> N                  | air <sup>a</sup>                      | 0.4            |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | C <sub>6</sub> D <sub>6</sub>                    | air <sup>a</sup>                      | 0.34           |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.7; λ <sub>exc</sub> = 347 nm.<br>f <sub>Δ</sub> <sup>T</sup> = 0.5 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 87R185           |
|   | C <sub>6</sub> H <sub>6</sub>                    | air <sup>a</sup>                      | 0.40*          |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.32; λ <sub>exc</sub> = 347 nm.<br>f <sub>Δ</sub> <sup>T</sup> = 1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 87R185           |
|   | CCl <sub>4</sub>                                 | O <sub>2</sub>                        | 0.6            |                             | MP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7. Used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; supersedes [79A010], [77E617], [78E881].  | 85F517           |
|   | D <sub>2</sub> O (mic)                           | air <sup>a</sup>                      | 0.11           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. cont. 2% Triton X-100  | 90E324           |
|   | D <sub>2</sub> O/EtOH (95:5)                     | air <sup>a</sup>                      | <0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90E324           |
|   | MeOD   | air <sup>a</sup>                      | 0.2            |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; meas. Φ <sub>T</sub> (S) = 0.22; λ <sub>exc</sub> = 347 nm.<br>f <sub>Δ</sub> <sup>T</sup> = -1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 87R185           |
| <b>2.2 Bacteriochlorophyll <i>b</i></b> |  |                                       |                |                             |             |  |                  |
|   | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup>                      | 0.48           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | C <sub>5</sub> H <sub>5</sub> N                  | air <sup>a</sup>                      | 0.43           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | CCl <sub>4</sub>                                 | O <sub>2</sub>                        | 0.65           |                             | MP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.   | 85F517           |
|   | D <sub>2</sub> O (mic)                           | air <sup>a</sup>                      | 0.15           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. cont. 2% Triton X-100.   | 90E324           |
|   | D <sub>2</sub> O/EtOH (95:5)                     | air <sup>a</sup>                      | <0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90E324           |
| <b>2.3 Chlorophyll <i>a</i></b>         |  |                                       |                |                             |             |  |                  |
|   | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup>                      | 0.52           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | i-C <sub>5</sub> H <sub>11</sub> OH              | air <sup>a</sup>                      | 0.77           |                             | CP/Oc-14    | A = ATU; λ <sub>exc</sub> = 436 nm.  | 56F007           |
|   | C <sub>5</sub> H <sub>5</sub> N                  | air <sup>a</sup>                      | 0.59           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90E324           |
|   | C <sub>5</sub> H <sub>5</sub> N                  | O <sub>2</sub>                        | 0.49           |                             | CP/Oc-14    | A = H <sub>2</sub> NCSNH <sub>2</sub> ; λ <sub>exc</sub> = 430 nm. Assumed f <sub>r</sub> <sup>A</sup> = 2.  | 737347<br>74E522 |
|   | c-C <sub>6</sub> H <sub>11</sub> OH              | air <sup>a</sup>                      | 0.77           |                             | CP/Oc-14    | A = ATU; λ <sub>exc</sub> = 436 nm.  | 56F007           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH | air <sup>a</sup>                      | 0.77           |                             | CP/Oc-14    | A = ATU; λ <sub>exc</sub> = 436 nm.  | 56F007           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>    | air <sup>a</sup>                      | 0.60           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>    | 8.5 × 10 <sup>-3</sup>                | 0.68           |                             | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50. Rel. to S' in MeOH.  | 84F191           |
|   | C <sub>6</sub> H <sub>6</sub>                    | 9.1 × 10 <sup>-3</sup>                | 0.60           |                             | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50. Rel. to S' in MeOH.  | 84F191           |
|   | CCl <sub>4</sub>                                 | air                                   | 0.57           |                             | MP/LI-56    | S' = Ph a. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; reported 0.55 in [79A010]; recalc'd. in [90R045] rel. to Φ <sub>Δ</sub> (TPP) = 0.70.  | 79A010<br>90R045 |
|   | CH <sub>3</sub> CN                               | air <sup>a</sup>                      | 0.60           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |
|   | D <sub>2</sub> O (mic)                           | air <sup>a</sup>                      | 0.35           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. cont. 2% Triton X-100.   | 90E324           |
|   | D <sub>2</sub> O/EtOH (95:5)                     | air <sup>a</sup>                      | <0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90E324           |
|   | H <sub>2</sub> O (mic)<br>pH = 7.0               | air                                   | 0.70-0.85      |                             | CP/Oc-14    | A = Im; P = Imidazole endoperoxide; λ <sub>exc</sub> = 660 nm. Soln. contg. 1% Triton X-100; assumed f <sub>r</sub> <sup>A</sup> = 0.17-0.2.   | 79N115           |
|   | MeOH   | air <sup>a</sup>                      | 0.77           |                             | CP/Oc-14    | A = ATU; λ <sub>exc</sub> = 436 nm.  | 56F007           |
| <b>2.4 Chlorophyll <i>b</i></b>         |  |                                       |                |                             |             |  |                  |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>    | air <sup>a</sup>                      | 0.75           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |
|   | C <sub>6</sub> D <sub>6</sub>                    | 1.2% O <sub>2</sub> in N <sub>2</sub> |                | 0.92                        | PR/LI-60    | S' = Np; TD = BP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for energy transfer efficiency.   | 91A358           |
|   | CH <sub>3</sub> CN                               | air <sup>a</sup>                      | 0.85           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]      | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment  | Ref.   |
|------|--|------------------------|----------------|-----------------------------|-------------|--|--------|
| 2.5  | Chlorophyll (oil soluble)  |                        |                |                             |             |  |        |
|      | C <sub>6</sub> H <sub>6</sub>  | 9.1 × 10 <sup>-3</sup> | 0.50           |                             | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50. Rel. to S' in MeOH.  | 84F191 |
| 2.6  | [22]COPROPORPHYRIN II  |                        |                |                             |             |  |        |
|      | CH <sub>2</sub> Cl <sub>2</sub>  | air <sup>a</sup>       | 1.1            |                             | CP/Pa-43    | S' = RB; A = 2,5-DMF; rel. to Φ <sub>Δ</sub> (S') = 0.80 <sup>b</sup> .  | 90R215 |
| 2.7  | Methyl acetal of oxidized octaethylporpurin ethyl ester  |                        |                |                             |             |  |        |
|      | MeOH   | air                    | 0.4            |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.64; meas. Φ <sub>T</sub> (S) = 0.6. f <sub>Δ</sub> <sup>T</sup> = 0.7 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; secondary Φ <sub>Δ</sub> (S') = 0.41, S' = ZnPCS.    | 90E491 |
| 2.8  | Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)-  |                        |                |                             |             |  |        |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       | 0.15*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.   | 90R204 |
|      |  |                        | 0.17           |                             |             |  |        |
| 2.9  | Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)-, chloroaluminum(III)   |                        |                |                             |             |  |        |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       | 0.37*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.   | 90R204 |
|      |  |                        | 0.42           |                             |             |  |        |
| 2.10 | Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)-, copper(II)  |                        |                |                             |             |  |        |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       | 0              |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm. Not detectable.   | 90R204 |
| 2.11 | Naphthalocyanine, bis(trihexylsilanolato)silicon (SiNC)  |                        |                |                             |             |  |        |
|      | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>         | 0.35           |                             | PL/LI-56    | S' = Np; rel. to Φ <sub>Δ</sub> (S') = 0.55; meas. Φ <sub>T</sub> (S) = 0.39; λ <sub>exc</sub> = 355 nm.   | 87R032 |
|      | C <sub>6</sub> D <sub>6</sub>  | air                    | 0.19           |                             | PL/LI-56    | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.29; meas. Φ <sub>T</sub> (S) = 0.20; λ <sub>exc</sub> = 355 nm.   | 88E657 |
| 2.12 | Pheophytin <i>a</i>  |                        |                |                             |             |  |        |
|      | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air                    | 0.67           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 90R045 |
|      | C <sub>5</sub> H <sub>5</sub> N  | O <sub>2</sub>         | 0.64           |                             | CP/Oc-14    | A = H <sub>2</sub> NCSNH <sub>2</sub> . Used f <sub>r</sub> <sup>A</sup> = 2.  | 74E522 |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.73           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543 |
|      | CCl <sub>4</sub>   | air                    | 0.71*          |                             | MP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 90R045 |
|      |  |                        | 0.80           |                             |             |  | 79A010 |
|      | CH <sub>3</sub> CN   | air <sup>a</sup>       | 0.85           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543 |
|      | D <sub>2</sub> O/EtOH<br>(90:10)<br>(mic)  | air                    | 0.70           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. Soln. cont. 2% Triton X-100.   | 90R045 |
|      | D <sub>2</sub> O/EtOH<br>(95:5)  | air                    | <0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90R045 |
|      | EtOH   | air                    | 0.60           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90R045 |
| 2.13 | Pheophytin <i>b</i>  |                        |                |                             |             |  |        |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.70           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543 |
|      | CH <sub>3</sub> CN   | air <sup>a</sup>       | 0.84           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543 |
| 2.14 | 20-Phorbinecarboxylic acid, 3,4-didehydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester (Octaethylidihydroporphyrin ethyl ester) |                        |                |                             |             |  |        |
|      | MeOII  | air                    | 0.71           |                             | PL/LI-56,42 | S' = IIP; rel. to Φ <sub>Δ</sub> (S') = 0.64; meas. Φ <sub>T</sub> (S) = 0.86. f <sub>Δ</sub> <sup>T</sup> = 0.83 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; secondary Φ <sub>Δ</sub> (S') = 0.41, S' = ZnPCS. | 90E491 |
| 2.15 | 20-Phorbinecarboxylic acid, 3,4-didehydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester, dichlorotin(IV)                         |                        |                |                             |             |  |        |
|      | MeOH   | air                    | 0.82           |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.64; meas. Φ <sub>T</sub> (S) = 0.96. f <sub>Δ</sub> <sup>T</sup> = 0.85 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; secondary Φ <sub>Δ</sub> (S') = 0.41, S' = ZnPCS.  | 90E491 |
| 2.16 | 20-Phorbinecarboxylic acid, 3,4,20,21-tetrahydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester (Octaethylporpurin, ethyl ester)  |                        |                |                             |             |  |        |
|      | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>       | 0.70           |                             | PL/LI-56,42 | S' = BChl a; rel. to Φ <sub>Δ</sub> (S') = 0.35; meas. Φ <sub>T</sub> (S) = 0.81; λ <sub>exc</sub> = 694 nm. f <sub>Δ</sub> <sup>T</sup> = 0.86 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.                     | 88R200 |
|      | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>       | 0.74*          |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.81; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.80 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.                         | 88R200 |
|      |  |                        | 0.65           |                             |             |  |        |
|      | MeOH   | air                    | 0.68           |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.64; meas. Φ <sub>T</sub> (S) = 0.82. f <sub>Δ</sub> <sup>T</sup> = 0.83 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; secondary Φ <sub>Δ</sub> (S') = 0.41, S' = ZnPCS.  | 90E491 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent          | [O <sub>2</sub> ] | $\phi_{\Delta}$ | $f_{\Delta}^T$   | Method | Comment | Ref. |
|--|------------------|-------------------|-----------------|--|--------|---------|------|
| <b>2.17 20-Phorbinecarboxylic acid, 3,4,20,21-tetrahydro-4,9,14,19-tetraethyl-18,19-dihydro-3,8,13,18-tetramethyl-, ethyl ester, zinc(II) (Etiopurpurin ethyl ester, zinc(II))</b>                     |                  |                   |                 |  |        |         |      |
| C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup> | 0.54              | PL/LI-56,42     | S' = BChl a; rel. to $\phi_{\Delta}(S') = 0.35$ ; meas. $\phi_T(S) = 0.84$ ; $\lambda_{exc} = 694$ nm. $f_{\Delta}^T = 0.71$ assuming $P_S^{O_2} = 0$ ; $P_T^{O_2} = 1$ .    |        | 88R200  |      |
| C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup> | 0.68*             | PL/LI-56,42     | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.84$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.64$ assuming $P_S^{O_2} = 0$ ; $P_T^{O_2} = 1$ .        |        | 88R200  |      |
| <b>2.18 3-Phorbinepropanoic acid, 9-acetyl-14-ethyl-13,14-dihydro-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester (Bacteriopheophytin <i>a</i>)</b>      |                  |                   |                 |  |        |         |      |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup> | 0.48              | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm.   |        | 90E324  |      |
| C <sub>5</sub> H <sub>5</sub> N  | air <sup>a</sup> | 0.8               | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm.   |        | 90E324  |      |
| C <sub>6</sub> D <sub>6</sub>  | air <sup>a</sup> | 0.53*             | PL/LI-56,42     | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.8$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.6$ assuming $P_S^{O_2} = 0$ ; used $P_T^{O_2} = 1$ .     |        | 87R185  |      |
| C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup> | 0.46              | PL/LI-56,42     | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.73$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.63$ assuming $P_S^{O_2} = 0$ ; used $P_T^{O_2} = 1$ .   |        | 87R185  |      |
| CCl <sub>4</sub>   | O <sub>2</sub>   | 0.75              | MP/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.7$ .  |        | 85F517  |      |
| CCl <sub>4</sub>   | air              | 0.69              | MP/LI-56        | S' = Chl a; rel. to $\phi_{\Delta}(S') = 0.55$ . $P_T^{O_2} = 1$ .   |        | 79A010  |      |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.36              | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm. Soln. cont. 2% Triton X-100.   |        | 90E324  |      |
| D <sub>2</sub> O/EtOH (95:5)   | air <sup>a</sup> | <0.02             | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm.  |        | 90E324  |      |
| MeOD   | air <sup>a</sup> | 0.2-0.3           | PL/LI-56,42     | S' = HP; rel. to $\phi_{\Delta}(S') = 0.53$ ; meas. $\phi_T(S) = 0.6$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.4-0.5$ assuming $P_S^{O_2} = 0$ ; used $P_T^{O_2} = 1$ . |        | 87R185  |      |
| <b>2.19 3-Phorbinepropanoic acid, 9-acetyl-14-ethylidene-13,14-dihydro-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester (Bacteriopheophytin <i>b</i>)</b> |                  |                   |                 |  |        |         |      |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup> | 0.43              | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm. Used $P_T^{O_2} = 1$ .  |        | 90E324  |      |
| C <sub>5</sub> H <sub>5</sub> N  | air <sup>a</sup> | 0.50              | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm.   |        | 90E324  |      |
| CCl <sub>4</sub>   | O <sub>2</sub>   | 0.75              | MP/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.7$ .  |        | 85F517  |      |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.35              | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm. Soln. cont. 2% Triton X-100.   |        | 90E324  |      |
| D <sub>2</sub> O/EtOH (95:5)   | air <sup>a</sup> | <0.02             | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 337$ nm.  |        | 90E324  |      |
| <b>2.20 3-Phorbinepropanoic acid, 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, magnesium(II) (Protocultiphophyllide)</b>                                       |                  |                   |                 |  |        |         |      |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air <sup>a</sup> | 0.77              | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ .   |        | 88F450  |      |
| D <sub>2</sub> O   | air <sup>a</sup> | ≤0.02             | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . Colloidal soln. contg. 0.5% NH <sub>4</sub> OH.  |        | 88F450  |      |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.84              | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . Soln. cont. 1% Triton X-100.   |        | 88F450  |      |
| <b>2.21 3-Phorbinepropanoic acid, 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester (Protopheophytin)</b>                 |                  |                   |                 |  |        |         |      |
| C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup> | 0.70              | PL/LI-56        | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm.  |        | 87E543  |      |
| CCl <sub>4</sub>   | air              | 0.88              | MP/LI-56        | S' = Chl a; rel. to $\phi_{\Delta}(S') = 0.55$ . $P_T^{O_2} = 1$ .   |        | 79A010  |      |
| CH <sub>3</sub> CN   | air <sup>a</sup> | 0.87              | PL/LI-56        | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm.  |        | 87E543  |      |
| <b>2.22 3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,6,13,18-tetramethyl-20-oxo- (Pheophorbide a)</b>   |                  |                   |                 |  |        |         |      |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O  | air              | 0.74              | PL/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ . $P_T^{O_2} = 1$ .   |        | 90R045  |      |
| CCl <sub>4</sub>   | air              | 0.71*             | MP/LI-56        | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ . $P_T^{O_2} = 1$ .   |        | 90R045  |      |
| D <sub>2</sub> O/EtOH (90:10) (mic)  | air              | 0.70              | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . $P_T^{O_2} = 1$ . Soln. cont. 2% Triton X-100.   |        | 90R045  |      |
| D <sub>2</sub> O/EtOH (95:5) (mic)   | air              | 0.49              | PL/LI-56        | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . $P_T^{O_2} = 1$ . Soln. cont. 2% Triton X-100.   |        | 90R045  |      |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent   | [O <sub>2</sub> ] | ϕ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment  | Ref.             |
|---|---|-------------------|----------------|-----------------------------|-------------|--|------------------|
| <b>2.22 3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,6,13,18-tetramethyl-20-oxo- (Pheophorbide a)—Continued</b>  |   |                   |                |                             |             |  |                  |
|   | D <sub>2</sub> O/EtOH<br>(95:5)                 | air               | <0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90R045           |
|   | EtOH  | air               | 0.60           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90R045           |
|   | EtOH  | air <sup>a</sup>  | 0.51           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 514.5 nm.  | 90R204           |
| <b>2.23 3-Phorbinepropanoic acid, [3,7,11,15-tetramethyl-2-hexadecenyl] 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoatomagnesium (Protochlorophyll)</b> |   |                   |                |                             |             |  |                  |
|   | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O | air <sup>a</sup>  | 0.84           |                             | PL/LI-56    | S' = TPP; rel. to ϕ <sub>Δ</sub> (S') = 0.70.  | 88F450           |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>  | 0.68           |                             | PL/LI-56    | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |
|   | CCl <sub>4</sub>                                | air               | 0.63           |                             | MP/LI-56    | S' = Chl a; rel. to ϕ <sub>Δ</sub> (S') = 0.55. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 79A010           |
|   | CH <sub>3</sub> CN                              | air <sup>a</sup>  | 0.78           |                             | PL/LI-56    | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.  | 87E543           |
|   | D <sub>2</sub> O                                | air <sup>a</sup>  | ≤0.02          |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70. Colloidal soln. contg. 0.5% NH <sub>4</sub> OH.   | 88F450           |
|   | D <sub>2</sub> O (mic)                          | air <sup>a</sup>  | 0.84           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70. Soln. cont. 1% Triton X-100.  | 88F450           |
| <b>2.24 Phthalocyanine, magnesium(II)</b>   |   |                   |                |                             |             |  |                  |
|   | C <sub>5</sub> H <sub>5</sub> N                 | O <sub>2</sub>    | 0.40           |                             | CP/Oc-14    | A = H <sub>2</sub> NCSNH <sub>2</sub> ; λ <sub>exc</sub> = 669 nm. Assumed f <sub>r</sub> <sup>A</sup> = 2.  | 737347<br>74E522 |
| <b>2.25 Phthalocyanine, zinc(II), bis(pyridine)</b>   |   |                   |                |                             |             |  |                  |
|   | C <sub>6</sub> H <sub>6</sub>                   | O <sub>2</sub>    | 0.50           |                             | PL/LI-56    | S' = ZnTPP; rel. to ϕ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 600 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.95.   | 89N079<br>90N126 |
|   | D <sub>2</sub> O (ves)<br>pD = 7.4              | O <sub>2</sub>    | 0.49           |                             | PL/LI-56    | S' = UP; rel. to ϕ <sub>Δ</sub> (S') = 0.71; λ <sub>exc</sub> = 600 nm. [DPPC] = 6.7 × 10 <sup>-4</sup> mol L <sup>-1</sup> , S' in D <sub>2</sub> O-Tris buffer.  | 90N126           |
|   | D <sub>2</sub> O (ves)<br>pD = 7.4              | O <sub>2</sub>    | 0.47           |                             | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.72; λ <sub>exc</sub> = 600 nm. [DPPC] = 6.7 × 10 <sup>-4</sup> mol L <sup>-1</sup> , S' in D <sub>2</sub> O-Tris buffer.  | 90N126           |
|   | EtOH  | air               | 0.53           |                             | CP/Ac-14    | A = DPBF; λ <sub>exc</sub> = 600 nm. Extrapolated to [A] → ∞.  | 88A284           |
|   | EtOH  | air               | 0.4            |                             | PL/LI-56    | S' = An; rel. to ϕ <sub>Δ</sub> (S') = 0.53; λ <sub>exc</sub> = 354 nm.  | 88A284           |
|   | EtOH  | air               | 0.4            |                             | PL/LI-56    | S' = ZnTPP; rel. to ϕ <sub>Δ</sub> (S') = 0.55; λ <sub>exc</sub> = 600 nm.   | 88A284           |
|   | H <sub>2</sub> O (ves)                          | air               | 0.7            |                             | CP/Ac-14    | A = DPBF; λ <sub>exc</sub> = 600 nm. Extrapolated to [A] → ∞; unilamellar DPPC vesicles.   | 88A284           |
| <b>2.26 Phthalocyanine, 1,4,8,11,15,18,22,25-octabutoxy-, zinc(II)</b>  |   |                   |                |                             |             |  |                  |
|   | C <sub>6</sub> D <sub>6</sub>                   | air               | 0.45           |                             | PL/LI-56    | S' = BP; rel. to ϕ <sub>Δ</sub> (S') = 0.29; meas. ϕ <sub>T</sub> (S) = 0.46; λ <sub>exc</sub> = 532 nm. Soln. cont. 1% pyridine.  | 89E453           |
|   | C <sub>6</sub> D <sub>6</sub>                   | air               | 0.50           |                             | PL/LI-56    | S' = BP; rel. to ϕ <sub>Δ</sub> (S') = 0.29; meas. ϕ <sub>T</sub> (S) = 0.52; λ <sub>exc</sub> = 532 nm. Soln. cont. 0.01% morpholine.   | 89E453           |
| <b>2.27 Phthalocyanine, sulfo- (mixed di-, tri- and tetrasulfo)</b>   |   |                   |                |                             |             |  |                  |
|   | D <sub>2</sub> O (mic)                          | air <sup>a</sup>  | 0.1            |                             | PL/LI-56,42 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.67; meas. ϕ <sub>T</sub> (S) = 0.25; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.4 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. Soln. cont. 0.01 mol L <sup>-1</sup> CTAB.                                  | 86F541<br>87R188 |
|   | H <sub>2</sub> O pH = 7                         | air               | 0.14           |                             | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to ϕ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 670 nm. RNO as monitor of P; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, ϕ <sub>Δ</sub> (S') at λ <sub>exc</sub> = 550 nm, cor. to 670 nm.   | 86R060           |
|   | H <sub>2</sub> O/MeOH<br>(1:1) pH = 7           | O <sub>2</sub>    | 0.12           |                             | CP/Pa-14    | A = TrpH; λ <sub>exc</sub> = 688 nm.   | 87F104           |
|   | H <sub>2</sub> O/MeOH<br>(1:1) pH = 7           | O <sub>2</sub>    | 0.10           |                             | CP/Pa-14    | A = TrpH; λ <sub>exc</sub> = 654 nm.   | 87F104           |
|   | MeOD  | air <sup>a</sup>  | 0.21*          |                             | PL/LI-56,42 | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.22; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.93 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using ϕ <sub>Δ</sub> (S') = 0.64 from [88Z155]. | 87R185<br>87R188 |
|   | MeOD  | air <sup>a</sup>  | 0.1            |                             | PL/LI-56,42 | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.22; λ <sub>exc</sub> = 694 nm. f <sub>Δ</sub> <sup>T</sup> = 0.6 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 87R185           |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent   | [O <sub>2</sub> ] | $\phi_{\Delta}$ | $f_{\Delta}^T$ | Method      | Comment   | Ref.             |
|------|---|-------------------|-----------------|----------------|-------------|---|------------------|
| 2.28 | <b>Phthalocyanine, trisulfo-, chloroaluminum(III)</b>     |                   |                 |                |             |   |                  |
|      | D <sub>2</sub> O pH = 7                                   | O <sub>2</sub>    | 0.34            |                | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.62$ ; meas. $\phi_T(S) = 0.46$ ; $\lambda_{exc} = 355$ nm. Rel. to S' in H <sub>2</sub> O; soln. contg. 2 × 10 <sup>-3</sup> mol L <sup>-1</sup> phosphate buffer and 1% NaCl wt/wt.; $P_T^{O_2} = 1$ . | 90A022<br>89R092 |
| 2.29 | <b>Phthalocyanine, sulfo-, chloroaluminum(III)</b>        |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0.34            |                | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
| 2.30 | <b>Phthalocyanine, sulfo-, aluminum(III)</b>              |                   |                 |                |             |   |                  |
|      | MeOD  | air <sup>a</sup>  | 0.36            |                | PL/LI-56,42 | S' = HP; rel. to $\phi_{\Delta}(S') = 0.64$ ; meas. $\phi_T(S) = 0.42$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.86$ assuming $P_S^{O_2} = 0$ .   | 91R242<br>87R188 |
| 2.31 | <b>Phthalocyanine, sulfo(phthalimido)-, aluminum(III)</b> |                   |                 |                |             |   |                  |
|      | MeOD  | air <sup>a</sup>  | 0.36            |                | PL/LI-56    | S' = HP; rel. to $\phi_{\Delta}(S') = 0.64$ ; $\lambda_{exc} = 347$ nm.   | 91R242           |
| 2.32 | <b>Phthalocyanine, sulfo-, cobalt(II)</b>                 |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0               |                | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
| 2.33 | <b>Phthalocyanine, sulfo-, copper(II)</b>                 |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0               |                | CP/Pa-43    | S' = RR; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
|      | H <sub>2</sub> O/MeOH (1:1) pH = 7                        | O <sub>2</sub>    | 0.12            |                | CP/Pa-14    | A = TrpH; $\lambda_{exc} = 668$ nm.   | 87F104           |
| 2.34 | <b>Phthalocyanine, sulfo-, iron(II)</b>                   |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0               |                | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
| 2.35 | <b>Phthalocyanine, tetrasulfo-, chlorogallium(III)</b>    |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O/MeOH (1:1) pH = 7                        | O <sub>2</sub>    | 0.47            |                | CP/Pa-14    | A = TrpH; $\lambda_{exc} = 680$ nm.   | 87F104           |
| 2.36 | <b>Phthalocyanine, sulfo-, chlorogallium(III)</b>         |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O/MeOH (1:1) pH = 7                        | O <sub>2</sub>    | 0.56            |                | CP/Pa-14    | A = TrpH; $\lambda_{exc} = 680$ nm.   | 87F104           |
| 2.37 | <b>Phthalocyanine, sulfo-, oxovanadium(IV)</b>            |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0               |                | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
| 2.38 | <b>Phthalocyanine, trisulfo-, zinc(II)</b>                |                   |                 |                |             |   |                  |
|      | D <sub>2</sub> O pH = 7                                   | O <sub>2</sub>    | 0.36            |                | PL/LI-56    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.62$ ; meas. $\phi_T(S) = 0.51$ ; $\lambda_{exc} = 355$ nm. Rel. to S' in H <sub>2</sub> O; soln. contg. 2 × 10 <sup>-3</sup> mol L <sup>-1</sup> phosphate buffer and 1% NaCl wt/wt.; $P_T^{O_2} = 1$ . | 90A022           |
| 2.39 | <b>Phthalocyanine, sulfo-, zinc(II)</b>                   |                   |                 |                |             |   |                  |
|      | H <sub>2</sub> O pH = 7                                   | air               | 0.45            |                | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 670$ nm. RNO as monitor of P; used $P_T^{O_2} = 1$ , $\phi_{\Delta}(S')$ at $\lambda_{exc} = 550$ nm, cor. to 670 nm.  | 86R060           |
|      | H <sub>2</sub> O/MeOH (1:1) pH = 7                        | O <sub>2</sub>    | 0.62            |                | CP/Pa-14    | A = TrpH; $\lambda_{exc} = 669$ nm.   | 87F104           |
|      | MeOD  | air <sup>a</sup>  | 0.43*           |                | PL/LI-56,42 | S' = HP; rel. to $\phi_{\Delta}(S') = 0.53$ ; meas. $\phi_T(S) = 0.56$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.78$ assuming $P_S^{O_2} = 0$ . $P_T^{O_2} = 1$ ; recalcd. using $\phi_{\Delta}(S') = 0.64$ from [88Z155].  | 87R188<br>87R185 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment   | Ref.   |
|---|---|-------------------|----------------|-----------------------------|-------------|---|--------|
| <b>2.39 Phthalocyanine, sulfo-, zinc(II)—Continued</b>  |   |                   |                |                             |             |   |        |
|   | MeOD  | air <sup>a</sup>  | 0.50*          |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; meas. Φ <sub>T</sub> (S) = 0.56; λ <sub>exc</sub> = 694 nm.<br>f <sub>Δ</sub> <sup>T</sup> = 0.88 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using Φ <sub>Δ</sub> (S') = 0.64 from [88Z155]. | 87R185 |
|   |   |                   | 0.41           |                             |             |   |        |
|   | MeOD  | air <sup>a</sup>  | 0.38*          |                             | PL/LI-56,42 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; meas. Φ <sub>T</sub> (S) = 0.56; λ <sub>exc</sub> = 650 nm.<br>f <sub>Δ</sub> <sup>T</sup> = 0.69 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using Φ <sub>Δ</sub> (S') = 0.64 from [88Z155]. | 86F541 |
|   |   |                   | 0.32           |                             |             |   |        |
| <b>2.40 Phthalocyanine, tetracarboxy-, copper(II)</b>   |   |                   |                |                             |             |   |        |
|   | DMSO  | O <sub>2</sub>    | 0.16           |                             | CP/Ac-15    | A = DPBF. Independent of [S] = (2-26) × 10 <sup>-6</sup> mol L <sup>-1</sup> ; dimers and oligomers may be present.   | 89F260 |
| <b>2.41 Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)-</b>  |   |                   |                |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air               | 0.15*          |                             | MP/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70.   | 90F095 |
|   |   |                   | 0.17           |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air <sup>a</sup>  | 0.14*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.  | 90R204 |
|   |   |                   | 0.16           |                             |             |   |        |
| <b>2.42 Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)-, chloroaluminum(III)</b>   |   |                   |                |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air <sup>a</sup>  | 0.28*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.  | 90R204 |
|   |   |                   | 0.31           |                             |             |   |        |
| <b>2.43 Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)-, copper(II)</b>  |   |                   |                |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air <sup>a</sup>  | 0.12*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.  | 90R204 |
|   |   |                   | 0.13           |                             |             |   |        |
| <b>2.44 Phthalocyanine, [2,9,16,23-tetrakis(1,1-dimethylethyl)]-, magnesium(II)</b>   |   |                   |                |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air <sup>a</sup>  | 0.06*          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 652 nm.  | 90R204 |
|   |   |                   | 0.07           |                             |             |   |        |
| <b>2.45 Phthalocyanine, tetrakis[methylenethio(dimethylamino)methylidyne]tetrakis[N-methylmethanaminiumato]-, copper(II), tetrachloride</b> |   |                   |                |                             |             |   |        |
|   | H <sub>2</sub> O pH = 7                       | air               | 0              |                             | CP/Pa-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 670 nm. RNO as monitor of P; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, Φ <sub>Δ</sub> (S') at λ <sub>exc</sub> = 550 nm, cor. to 670 nm.  | 86R060 |
| <b>2.46 Porphine</b>  |   |                   |                |                             |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>  | 0.67           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504 |
|   | CCl <sub>4</sub>                              | air               | 0.75           |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F161 |
| <b>2.47 Porphine-21,23-d<sub>2</sub></b>  |   |                   |                |                             |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>  | 0.70           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90E615 |
| <b>2.48 Porphine, 5-amino-2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- (5-Aminoetioporphyrin I)</b>  |   |                   |                |                             |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>  | 0.85           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504 |
| <b>2.49 Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate</b>                           |   |                   |                |                             |             |   |        |
|   | D <sub>2</sub> O/EtOH                         | air <sup>a</sup>  | 0.49           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 337 nm. Rel. to TPP in CCl <sub>4</sub> , (7:3)   | 86F316 |
| <b>2.50 Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, cobalt(II)</b>               |   |                   |                |                             |             |   |        |
|   | D <sub>2</sub> O/EtOH                         | air <sup>a</sup>  | ≤0.02          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 337 nm. Rel. to TPP in CCl <sub>4</sub> , (7:3)   | 86F316 |
| <b>2.51 Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, manganese(II)</b>            |   |                   |                |                             |             |   |        |
|   | D <sub>2</sub> O/EtOH                         | air <sup>a</sup>  | ≤0.02          |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 337 nm. Rel. to TPP in CCl <sub>4</sub> , (7:3)   | 86F316 |
| <b>2.52 Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, zinc(II)</b>                 |   |                   |                |                             |             |   |        |
|   | D <sub>2</sub> O/EtOH                         | air <sup>a</sup>  | 0.24           |                             | PL/LI-56    | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 337 nm. Rel. to TPP in CCl <sub>4</sub> , (7:3)   | 86F316 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]                             | $\phi_{\Delta}$  | $f_{\Delta}^T$ | Method   | Comment   | Ref.   |
|------|--|---|------------------|----------------|----------|---|--------|
| 2.53 | Porphine, 21,23-dideutero-2,3-dihydro-5,10,15,20-tetraphenyl- (Tetraphenylchlorin- <i>d</i> <sub>2</sub> )                       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.70           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.54 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl- (Octaethylporphyrin- <i>d</i> <sub>2</sub> )                            | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.75           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.55 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-2,3-dihydro- (Octaethylchlorin- <i>d</i> <sub>2</sub> )                  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.60           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.56 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-5-methyl- ( $\alpha$ -Methyloctaethylporphyrin- <i>d</i> <sub>2</sub> )  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.81           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.57 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-21-methyl- ( <i>N</i> -Methyloctaethylporphyrin- <i>d</i> <sub>2</sub> ) | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.55           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.58 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-5-phenyl- ( $\alpha$ -Phenoxyoctaethylporphyrin- <i>d</i> <sub>2</sub> ) | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.60           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.59 | Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenyl-   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.67           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.60 | Porphine, 21,23-dideutero-2,3,12,13-tetraethyl-  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.72           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.61 | Porphine, 21,23-dideutero-2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- (Etioporphyrin- <i>d</i> <sub>2</sub> )                    | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.75           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.62 | Porphine, 21,23-dideutero-5,10,15,20-tetrakis(2-chlorophenyl)-   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.84           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.63 | Porphine, 21,23-dideutero-5,10,15,20-tetrakis(3-chlorophenyl)-   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.89           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.64 | Porphine, 21,23-dideutero-5,10,15,20-tetrakis(4-chlorophenyl)-   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.83           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.65 | Porphine, 21,23-dideutero-5,10,15,20-tetraphenyl- (TPP- <i>d</i> <sub>2</sub> )  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.86           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.66 | Porphine, 21,23-dideutero-5,10,15,20-tetrapropyl-  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.92           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ . | 90E615 |
| 2.67 | Porphine, 2,3-dihydro-5,10,15,20-tetraphenyl- (Tetraphenylchlorin, TPC)  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.65           | PL/LI-56 | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ .   | 89A504 |
|      |  | CCl <sub>4</sub>                              | air              | 0.55           | MP/LI-56 | S' = Ph a; rel. to $\phi_{\Delta}(S') = 0.8$ .  | 82F161 |
| 2.68 | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.80           | PL/LI-56 | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   | 91E392 |
|      |  | CCl <sub>4</sub>                              | air <sup>a</sup> |                | PL/LI-56 | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.80$ ; $\lambda_{exc} = 347$ nm.   | 91E392 |
| 2.69 | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, copper(II)   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.85           | PL/LI-56 | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   | 91E392 |
|      |  | CCl <sub>4</sub>                              | air <sup>a</sup> |                | PL/LI-56 | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.86$ ; $\lambda_{exc} = 347$ nm.   | 91E392 |
| 2.70 | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, copper(II)zinc(II)   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.35           | PL/LI-56 | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   | 91E392 |
|      |  | CCl <sub>4</sub>                              | air <sup>a</sup> |                | PL/LI-56 | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.36$ ; $\lambda_{exc} = 347$ nm.   | 91E392 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent  | [O <sub>2</sub> ]      | $\phi_{\Delta}$ | $f_{\Delta}^T$ | Method  | Comment | Ref.                       |
|------|--|------------------------|-----------------|----------------|---|---------|----------------------------|
| 2.71 | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, biszinc(II)    |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.88            | PL/LI-56       | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   |         | 91E392                     |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.70$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
| 2.72 | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octapropyl-, biscopper(II) |                        |                 |                |   |         |                            |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.09$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
| 2.73 | Porphine, 2,3,7,8,12,13,17,18-octaethyl- (Octaethylporphyrin, OEP)           |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.75            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ .   |         | 89A504<br>87E667           |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.75            | PL/LI-56       | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   |         | 91E392                     |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.72$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
| 2.74 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, cadmium(II) (CdOEP)                |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.80            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.75 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, copper(II)                         |                        |                 |                |   |         |                            |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
| 2.76 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, lead(II)                           |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.78            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.77 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, indium(II)                         |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.76            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.78 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, oxotitanium(IV)                    |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.80            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.79 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, oxovanadium(IV)                    |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.84            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.80 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, palladium(II)                      |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 1               |                | Reference value, same as PdMPDME, see 2.73, 2.83.   |         |                            |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.86$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
| 2.81 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, scandium(III)                      |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.88            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.82 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, dichlorotin(IV)                    |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | 1.8 × 10 <sup>-3</sup> | 0.40            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.                 |         | 87E667                     |
| 2.83 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-, zinc(II) (ZnOEP)                   |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.85            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ .   |         | 89A504<br>87E667<br>87E543 |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.85            | PL/LI-56       | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   |         | 91E392                     |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.72$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |
|      | CH <sub>3</sub> CN   | air <sup>a</sup>       | 0.75            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm.                   |         | 87E543                     |
| 2.84 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-2,3-dihydro-                         |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.60            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ .   |         | 89A504                     |
| 2.85 | Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl-                            |                        |                 |                |   |         |                            |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.74            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{Q_2} = 1$ . |         | 90E615                     |
|      | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>                                | air <sup>a</sup>       | 0.75            | PL/LI-56       | S' = PdOEP; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{exc} = 347$ nm.                   |         | 91E392                     |
|      | CCl <sub>4</sub>   | air <sup>a</sup>       |                 | PL/LI-56       | S' = GaTPP; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.77$ ; $\lambda_{exc} = 347$ nm.   |         | 91E392                     |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]      | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method         | Comment   | Ref.             |
|-------|--|------------------------|----------------|-----------------------------|----------------|---|------------------|
| 2.86  | Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl-, copper(II)                                  |                        |                |                             |                |   |                  |
|       | CCl <sub>4</sub>   | air <sup>a</sup>       |                |                             | PL/LI-56       | S' = GaTPP; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.25; λ <sub>exc</sub> = 347 nm.   | 91E392           |
| 2.87  | Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl-, zinc(II)                                    |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.85           |                             | PL/LI-56       | S' = PdOEP; rel. to Φ <sub>Δ</sub> (S') = 1 <sup>b</sup> ; λ <sub>exc</sub> = 347 nm.   | 91E392           |
|       | CCl <sub>4</sub>   | air <sup>a</sup>       |                |                             | PL/LI-56       | S' = GaTPP; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.78; λ <sub>exc</sub> = 347 nm.   | 91E392           |
| 2.88  | Porphine, 2,3,7,8,12,13,17,18-octaethyl-21-methyl-   |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.55           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.89  | Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-phenyl-  |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.54           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90E615           |
| 2.90  | Porphine, 2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenyl-                               |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.52           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.91  | Porphine, 2,3,7,8-tetraethyl-  |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.64           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.92  | Porphine, 2,3,12,13-tetraethyl-  |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.72           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.93  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- (Etioporphyrin I)                        |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | 1.8 × 10 <sup>-3</sup> | 0.75           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E667<br>89A504 |
| 2.94  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-, zinc(II)                                |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | 1.8 × 10 <sup>-3</sup> | 0.80           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E667<br>89A504 |
| 2.95  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10-dinitro-                             |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.33           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.96  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10-dinitro-, zinc(II)                   |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.44           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.97  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,15-dinitro-                             |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.31           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.98  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,15-dinitro-, zinc(II)                   |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.34           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.99  | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5-nitro-                                  |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.57           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.100 | Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10,15-trinitro-                         |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.36           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.101 | Porphine, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (E) (Tetraphenylbacteriochlorin, TPBC) |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | 1.8 × 10 <sup>-3</sup> | 0.48           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E667<br>89A504 |
|       | CCl <sub>4</sub>   | air                    | 0.45           |                             | MP/LI-56       | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8.   | 82F161           |
| 2.102 | Porphine, 5,10,15,20-tetrakis(4-bromophenyl)-  |                        |                |                             |                |   |                  |
|       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>  | air <sup>a</sup>       | 0.81           |                             | PL/LI-56       | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.  | 89A504           |
| 2.103 | Porphine, 5,10,15,20-tetrakis(4-carboxyphenyl)-  |                        |                |                             |                |   |                  |
|       | H <sub>2</sub> O   | air <sup>a</sup>       | 0.70           |                             | PL/LI,St-55,42 | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.51; meas. Φ <sub>T</sub> (S) = 0.76; λ <sub>exc</sub> = 532 nm.<br>Δε <sub>T</sub> (S) = 27,000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.53 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 | 86A407           |
|       | pH = 7.4   |                        |                |                             |                |   |                  |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]                             | ϕ <sub>Δ</sub>   | f <sub>Δ</sub> <sup>T</sup> | Method         | Comment  | Ref.   |
|-------|--|---|------------------|-----------------------------|----------------|--|--------|
| 2.103 | Porphine, 5,10,15,20-tetrakis(4-carboxyphenyl)—Continued                 |   |                  |                             |                |  |        |
|       | H <sub>2</sub> O pH = 7  | air   | 0.58             |                             | CP/Pa-43       | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = Im; P = Imidazole endoperoxide; rel. to ϕ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.  | 84F253 |
|       | H <sub>2</sub> O pH = 7  | air   | 0.58             |                             | CP/Oc-43       | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA.   | 84F253 |
|       | H <sub>2</sub> O (mic)   | air <sup>a</sup>                              | 0.98             | PL/LI,St-55,42              |                | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.67; meas. ϕ <sub>T</sub> (S) = 0.85; λ <sub>exc</sub> = 532 nm. Δε <sub>T</sub> (S) = 36,500 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; ϕ <sub>Δ</sub> = 0.83 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; soln. cont. 2% Triton X-100. | 86A407 |
| 2.104 | Porphine, 5,10,15,20-tetrakis(2-chlorophenyl)-                           | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.84                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.105 | Porphine, 5,10,15,20-tetrakis(3-chlorophenyl)-                           | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.81                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.106 | Porphine, 5,10,15,20-tetrakis(4-chlorophenyl)-                           | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.71                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.107 | Porphine, 5,10,15,20-tetrakis(2,6-dichloro-3-sulfonatophenyl)-, zinc(II) | H <sub>2</sub> O pH = 7                       | O <sub>2</sub>   | 0.74                        | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.62. ϕ <sub>Δ</sub> = 0.76 for dye bound with human serum albumin.   | 90R041 |
| 2.108 | Porphine, 5,10,15,20-tetrakis(2-fluorophenyl)-                           | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.71                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.109 | Porphine, 5,10,15,20-tetrakis(2-fluorophenyl)-, zinc(II)                 | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.93                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.110 | Porphine, 5,10,15,20-tetrakis(4-fluorophenyl)-                           | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.65                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.111 | Porphine, 5,10,15,20-tetrakis(2-hydroxyphenyl)-                          | MeOD  | air              | 0.65*                       | PL/LI-56,42    | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.68; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using ϕ <sub>Δ</sub> (S') = 0.64 from [88Z155].   | 88E519 |
|       |  |   |                  | 0.54                        |                |  |        |
| 2.112 | Porphine, 5,10,15,20-tetrakis(3-hydroxyphenyl)-                          | EtOH  | air <sup>a</sup> | 0.50                        | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 514,5 nm.  | 90R204 |
|       | MeOD   | air   | 0.69*            | PL/LI-56,42                 |                | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.69; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using ϕ <sub>Δ</sub> (S') = 0.64 from [88Z155].   | 88E519 |
|       |  |   | 0.57             |                             |                |  |        |
| 2.113 | Porphine, 5,10,15,20-tetrakis(4-hydroxyphenyl)- (T(p-HOP)P)              | EtOH  | air <sup>a</sup> | 0.58                        | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 514.5 nm.  | 90R204 |
|       | MeOD   | air   | 0.70*            | PL/LI-56,42                 |                | S' = HP; rel. to ϕ <sub>Δ</sub> (S') = 0.53; meas. ϕ <sub>T</sub> (S) = 0.65; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; recalcd. using ϕ <sub>Δ</sub> (S') = 0.64 from [88Z155].   | 88E519 |
|       |  |   | 0.56             |                             |                |  |        |
| 2.114 | Porphine, 5,10,15,20-tetrakis(4-iodophenyl)-                             | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup> | 0.97                        | PL/LI-56       | S' = PdMPDME; rel. to ϕ <sub>Δ</sub> (S') = 1.0.   | 89A504 |
| 2.115 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-2-yl)-                  | H <sub>2</sub> O pH = 7                       | air              | 0.68                        | CP/Oc or Pa-43 | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA, assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 86R162 |
| 2.116 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-3-yl)-                  | H <sub>2</sub> O pH = 7                       | air              | 0.77                        | CP/Oc or Pa-43 | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to ϕ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA, assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 86R162 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]     | $\phi_{\Delta}$ | $f_{\Delta}^T$ | Method         | Comment   | Ref.   |
|-------|---|-----------------------|-----------------|----------------|----------------|---|--------|
| 2.117 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)- (H <sub>2</sub> TMpyP <sup>4+</sup> ) |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.74            |                | CP/Oc-14       | A = FFA; $\lambda_{exc}$ = 436 nm. $P_T^{O_2}$ = 1.   | 84F253 |
| 2.118 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, cadmium(II)                          |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.75            |                | CP/Oc-43       | $S' = H_2\text{TMpyP}^{4+}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 546 nm.   | 84F253 |
| 2.119 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, cobalt(II)                           |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | <0.001          |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 436 or 546 nm. A = Im or FFA.  | 84F253 |
| 2.120 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, copper(II)                           |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | <0.001          |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 436 or 546 nm. A = Im or FFA.  | 84F253 |
| 2.121 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, iron(II)                             |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | <0.001          |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 436 or 546 nm. A = Im or FFA, assumed $P_T^{O_2}$ = 1.   | 86R162 |
| 2.122 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, lutetium(III)                        |                       |                 |                |                |   |        |
|       | D <sub>2</sub> O pD = 7 O <sub>2</sub>  |                       | 0.78            |                | PL/LI-56       | $S' = \text{AlPCS}$ ; rel. to $\phi_{\Delta}(S') = 0.34$ .  | 91E452 |
| 2.123 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, magnesium(II)                        |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.69            |                | CP/Oc-43       | $S' = H_2\text{TMpyP}^{4+}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 546 nm.   | 84F253 |
| 2.124 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, manganese(III)                       |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | <0.001          |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 436 or 546 nm. A = Im or FFA.  | 84F253 |
| 2.125 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, nickel(II)                           |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | <0.001          |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 436 or 546 nm. A = Im or FFA, assumed $P_T^{O_2}$ = 1.   | 86R162 |
| 2.126 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, palladium(II)                        |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.12            |                | CP/Oc-43       | $S' = H_2\text{TMpyP}^{4+}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 546 nm. $P_T^{O_2} \neq 1$ .  | 84F253 |
| 2.127 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, tin(IV)                              |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.78            |                | CP/Pa-43       | $S' = H_2\text{TMpyP}^{4+}$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 546 nm. RNO as monitor of P.   | 84F253 |
| 2.128 | Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, zinc(II)                             |                       |                 |                |                |   |        |
|       | H <sub>2</sub> O pH = 7 air   |                       | 0.88            |                | CP/Oc-43       | $S' = H_2\text{TMpyP}^{4+}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc}$ = 546 nm.   | 84F253 |
| 2.129 | Porphine, tetrakis(4-sulfonatophenyl)-  |                       |                 |                |                |   |        |
|       | D <sub>2</sub> O pH = 7 O <sub>2</sub>  |                       | 0.64            |                | PL/LI-56       | meas. $\phi_T(S) = 0.79$ ; $\lambda_{exc}$ = 532 nm. Rel. to $\phi_{\Delta} = 0.62$ for H <sub>2</sub> TPPS <sup>4-</sup> in H <sub>2</sub> O; soln. contg. $2 \times 10^{-3}$ mol L <sup>-1</sup> phosphate buffer and 1% NaCl wt/wt.; $P_T^{O_2} = 1$ . | 90A022 |
|       | D <sub>2</sub> O  | $2.45 \times 10^{-4}$ | 0.76            |                | PL/LI-56       | $S' = \text{PdTTPS}^{4-}$ ; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc}$ = 347 nm.   | 87E941 |
|       | D <sub>2</sub> O  | air <sup>a</sup>      | 0.42            |                | PL/LI-56       | $S' = \text{TPP}$ ; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc}$ = 337 nm. Rel. to TPP in CCl <sub>4</sub> .   | 86F316 |
|       | H <sub>2</sub> O pH = 7.4   | O <sub>2</sub>        | 0.71            |                | CP/Oc-14       | A = Im; $\lambda_{exc}$ = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.  | 88N170 |
|       | H <sub>2</sub> O pH = 7.4   | O <sub>2</sub>        | 0.33            |                | PL/Ac-14       | A = TrpH; $\lambda_{exc}$ = 630 nm. Soln. cont. 1.6% NaCl in phosphate buffer.  | 88N170 |
|       | H <sub>2</sub> O pH = 7.4   | O <sub>2</sub>        | 0.48            |                | CP/Pa-43       | $S' = \text{RB}$ ; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc}$ = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer; RNO as monitor for P.  | 88N170 |
|       | H <sub>2</sub> O pH = 7.4   | O <sub>2</sub>        | 0.50            |                | CP/Ac-14       | A = TrpH; $\lambda_{exc}$ = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.  | 88N170 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]                             | Φ <sub>Δ</sub>          | f <sub>Δ</sub> <sup>T</sup> | Method  | Comment  | Ref.             |
|-------|--|---|-------------------------|-----------------------------|---|--|------------------|
| 2.129 | Porphine, tetrakis(4-sulfonatophenyl)—Continued                    |   |                         |                             |   |  |                  |
|       | H <sub>2</sub> O<br>pH = 7.4                                       | air <sup>a</sup>                              | 1.3                     | PL/LI,St-55,42              | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.51; meas. Φ <sub>T</sub> (S) = 0.57; λ <sub>exc</sub> = 532 nm.<br>Δε <sub>T</sub> (S) = 52,000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.75 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.                              |  | 86A407           |
|       | H <sub>2</sub> O pH = 7  | air   | 0.62                    | CP/Oc or Pa-43              | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA.  |  | 84F253           |
|       | H <sub>2</sub> O pH = 7  | air   | 0.67                    | CP/Pa-43                    | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.   |  | 84F253           |
|       | H <sub>2</sub> O (mic)   | air <sup>a</sup>                              | 1.2                     | PL/LI,St-55,42              | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.67; meas. Φ <sub>T</sub> (S) = 0.65; λ <sub>exc</sub> = 532 nm.<br>Δε <sub>T</sub> (S) = 57,000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.80 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; soln. cont. 2% Triton X-100.  |  | 86A407           |
| 2.130 | Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, palladium(II)   | D <sub>2</sub> O                              | 2.45 × 10 <sup>-4</sup> | 1.0                         |   | λ <sub>exc</sub> = 347 nm. Φ <sub>T</sub> = 1; used as reference value.  | 87E941           |
| 2.131 | Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, dichlorotin(IV) | D <sub>2</sub> O pH = 7                       | O <sub>2</sub>          | 0.77                        | PL/LI-5G  | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.62; meas. Φ <sub>T</sub> (S) = 1.0; λ <sub>exc</sub> = 532 nm. Rel. to S' in H <sub>2</sub> O; soln. contg. 2 × 10 <sup>-3</sup> mol L <sup>-1</sup> phosphate buffer and 1% NaCl wt/wt.; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.                | 90A022           |
|       | H <sub>2</sub> O pH = 7  | air   | 0.67                    | CP/Oc or Pa-43              | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA, assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   |  | 86R162           |
| 2.132 | Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, ytterbium(II)   | H <sub>2</sub> O<br>pH = 7.0                  | O <sub>2</sub>          | 0.04                        | CP/Pa-43  | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.   | 89F580           |
| 2.133 | Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, zinc(II)        | D <sub>2</sub> O                              | 2.45 × 10 <sup>-4</sup> | 0.77                        | PL/LI-56  | S' = PdTPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.  | 87E941           |
| 2.134 | Porphine, 5,10,15,20-tetrakis(4-trimethylammoniophenyl)-           | H <sub>2</sub> O<br>pH = 7.4                  | air <sup>a</sup>        | 0.85                        | PL/LI,St-55,42  | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.51; meas. Φ <sub>T</sub> (S) = 0.56; λ <sub>exc</sub> = 532 nm.<br>Δε <sub>T</sub> (S) = 48,000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.48 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 86A407           |
|       | H <sub>2</sub> O pH = 7  | air   | 0.77                    | CP/Oc or Pa-43              | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 or 546 nm. A = Im or FFA.  |  | 84F253           |
|       | H <sub>2</sub> O pH = 7  | air   | 0.69                    | CP/Pa-43                    | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.   |  | 84F253           |
|       | H <sub>2</sub> O (mic)   | air <sup>a</sup>                              | 1.3                     | PL/LI,St-55,42              | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.67; meas. Φ <sub>T</sub> (S) = 0.58; λ <sub>exc</sub> = 532 nm.<br>Δε <sub>T</sub> (S) = 53,000 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.73 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; Soln. cont. 2% Triton X-100. |  | 86A407           |
| 2.135 | Porphine, 3,7,12,18-tetramethyl-2,8-diethyl-                       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>        | 0.67                        | PL/LI-56  | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0.   | 89A504           |
| 2.136 | Porphine, 5,10,15,20-tetraphenyl- (TPP)                            | C <sub>5</sub> H <sub>5</sub> N               | O <sub>2</sub>          | 0.74                        | CP/Oc-14  | A = H <sub>2</sub> NCSNH <sub>2</sub> ; λ <sub>exc</sub> = 430 nm. Assumed f <sub>r</sub> <sup>A</sup> = 2.  | 737347<br>74E522 |
|       | n-C <sub>3</sub> H <sub>7</sub> I                                  | air   | 0.77                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | c-C <sub>4</sub> H <sub>8</sub> O                                  | air   | 0.62                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | c-C <sub>6</sub> H <sub>12</sub>                                   | air   | 0.67                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> D <sub>5</sub> Br                                   | air   | 0.69                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> D <sub>6</sub>                                      | air   | 0.62                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> F <sub>5</sub> Br                                   | air   | 0.66                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> F <sub>5</sub> Cl                                   | air   | 0.57                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> F <sub>5</sub> I                                    | air   | 0.75                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |
|       | C <sub>6</sub> F <sub>6</sub>                                      | air   | 0.57                    | CP/Ac-14                    | A = DPBF.   | 90E215   |                  |

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]      | Φ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment   | Ref.   |
|---|---|------------------------|-------------------|-----------------------------|-------------|---|--------|
| <b>2.136 Porphine, 5,10,15,20-tetraphenyl- (TPP)—Continued</b>      |   |                        |                   |                             |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.1 × 10 <sup>-3</sup> | 0.69              |                             | PL/LI-56    | S' = PdTPP; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E941 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup> | 0.70              |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E667 |
|   |   |                        |                   |                             |             |   | 89A504 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 8.5 × 10 <sup>-3</sup> | 0.88              |                             | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50. Rel. to S' in MeOH.   | 84F191 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | O <sub>2</sub>         | 0.88              |                             | CP/Tr,St-51 | A = DPBF; λ <sub>exc</sub> = 546 nm; used ϕ <sub>F</sub> (S) = 0.05. Measured Φ <sub>ox</sub> = 0.88 and ΔH <sub>ox</sub> = -185 kJ mol <sup>-1</sup> .   | 80C002 |
|   | C <sub>6</sub> H <sub>5</sub> Br              | air                    | 0.69              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
|   | C <sub>6</sub> H <sub>5</sub> Cl              | air                    | 0.61              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
|   | C <sub>6</sub> H <sub>5</sub> F               | air                    | 0.60              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
|   | C <sub>6</sub> H <sub>5</sub> I               | air                    | 0.70              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 0.1 × 10 <sup>-3</sup> | 0.41 <sup>T</sup> | 0.71                        | PL/LI-56,38 | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83; λ <sub>exc</sub> = 532 nm; used ϕ <sub>T</sub> (S) = 0.63. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90A328 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.55              | 0.74                        | PL/LI-56,42 | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83; used ϕ <sub>T</sub> (S) = 0.63. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; assumed f <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90A328 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.62              |                             | CP/Ac-14    | A = DPBF. Ave. with value from [89E223].  | 90E215 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.67              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.72*             |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. ϕ <sub>T</sub> (S) = 0.67; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.92 assuming P <sub>T</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.        | 88E519 |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.63              |                             |             |   |        |
|   | C <sub>6</sub> H <sub>6</sub>                 | air                    | 0.58              |                             | PL/Hp-52    | λ <sub>exc</sub> = 590 nm.  | 85E591 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 9 × 10 <sup>-3</sup>   | 0.62              |                             | PL/LI-56    | S' = Pz; rel. to Φ <sub>Δ</sub> (S') = 0.83.  | 90A328 |
|   | C <sub>6</sub> H <sub>6</sub>                 | 9.1 × 10 <sup>-3</sup> | 0.89              |                             | CP/Oc-43    | S' = MB <sup>+</sup> ; A = TME; rel. to Φ <sub>Δ</sub> (S') = 0.50. Rel. to S' in MeOH.   | 84F191 |
|   | CCl <sub>4</sub>                              | air                    | 0.62              |                             |             | See Table 4.  |        |
|   | CCl <sub>4</sub>                              | air                    | 0.54              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | CCl <sub>4</sub>                              | air                    | 0.65              |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F161 |
|   | CCl <sub>4</sub>                              | air                    | 0.7               |                             | MP/LI-56    | S' not given, probably Chl a, Φ <sub>Δ</sub> = 0.55.  | 81E631 |
|   | CCl <sub>4</sub>                              | O <sub>2</sub>         | 0.88              |                             | CP/Tr-51    | λ <sub>exc</sub> = 546 nm. A = DPBF, 2,5-DMF and TME; measured ϕ <sub>F</sub> , Φ <sub>ox</sub> = 0.88 and ΔH <sub>ox</sub> = -205, -95, and -175 kJ mol <sup>-1</sup> for DPBF, 2,5-DMF and TME, resp.; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 80C002 |
|   | CH <sub>3</sub> CN                            | air                    | 0.60              |                             | CP/Ac-14    | A = DPBF. Ave. with value from [89E223].  | 90E215 |
|   | CH <sub>3</sub> CN                            | air                    | 0.50              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | CHCl <sub>3</sub>                             | air                    | 0.55              |                             | CP/Ac-14    | A = DPBF. Ave. with value from [89E223].  | 90E215 |
|   | CHCl <sub>3</sub>                             | air                    | 0.50              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | CS <sub>2</sub>                               | air                    | 0.51              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | ClCF <sub>2</sub> CCl <sub>2</sub> F          | air                    | 0.41              |                             | CP/Ac-14    | A = MDH. f <sub>r</sub> <sup>A</sup> = 0.30.  | 89E223 |
|   | ClCF <sub>2</sub> CCl <sub>2</sub> F          | O <sub>2</sub>         | ~1                |                             | CP/Tr-51    | A = DPBF; λ <sub>exc</sub> = 404 nm. Measured ϕ <sub>F</sub> (S) = 0.03, Φ <sub>ox</sub> = 1.0 and ΔH <sub>ox</sub> = -195 kJ mol <sup>-1</sup> ; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1   | 80C002 |
|   | 2-EtNp  | air                    | 0.63              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
|   | 1-MeNp  | air                    | 0.34              |                             | CP/Ac-14    | A = DPBF.   | 90E215 |
| <b>2.137 Porphine, tetraphenyl-, cadmium(II)</b>                    |   |                        |                   |                             |             |   |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup> | 0.96              |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E667 |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.1 × 10 <sup>-3</sup> | 0.98              |                             | PL/LI-56    | S' = PdTPP; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E941 |
| <b>2.138 Porphine, 5,10,15,20-tetraphenyl-, chloroaluminum(III)</b> |   |                        |                   |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air                    | 0.90              |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8.   | 82F161 |
| <b>2.139 Porphine, 5,10,15,20-tetraphenyl-, cobalt(II)</b>          |   |                        |                   |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air                    | <0.01             |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8.   | 82F161 |
| <b>2.140 Porphine, 5,10,15,20-tetraphenyl-, copper(II)</b>          |   |                        |                   |                             |             |   |        |
|   | CCl <sub>4</sub>                              | air                    | <0.01             |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8.   | 82F161 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent   | [O <sub>2</sub> ]      | $\phi_{\Delta}$   | $f_{\Delta}^T$ | Method         | Comment  | Ref.             |
|--|---|------------------------|-------------------|----------------|----------------|--|------------------|
| <b>2.141 Porphine, 5,10,15,20-tetraphenyl-, dichlorotin(IV)</b>  |   |                        |                   |                |                |  |                  |
|  | CCl <sub>4</sub>                                | air                    | 0.55              |                | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ .   | 82F161           |
| <b>2.142 Porphine, 5,10,15,20-tetraphenyl-, gallium(II)</b>  |   |                        |                   |                |                |  |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>       | 0.85              |                | PL/LI-56       | $S' = \text{PdOEP}$ ; rel. to $\phi_{\Delta}(S') = 1^b$ ; $\lambda_{\text{exc}} = 347 \text{ nm}$ .  | 91E392           |
| <b>2.143 Porphine, 5,10,15,20-tetraphenyl-, iron(III)</b>  |   |                        |                   |                |                |  |                  |
|  | CCl <sub>4</sub>                                | air                    | <0.01             |                | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ .   | 82F161           |
| <b>2.144 Porphine, 5,10,15,20-tetraphenyl-, manganese(III)</b>   |   |                        |                   |                |                |  |                  |
|  | CCl <sub>4</sub>                                | air                    | <0.01             |                | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ .   | 82F161           |
| <b>2.145 Porphine, 5,10,15,20-tetraphenyl-, nickel(II)</b>   |   |                        |                   |                |                |  |                  |
|  | CCl <sub>4</sub>                                | air                    | <0.01             |                | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ .   | 82F161           |
| <b>2.146 Porphine, 5,10,15,20-tetraphenyl-, zinc(II) (ZnTPP)</b>   |   |                        |                   |                |                |  |                  |
|  | C <sub>5</sub> H <sub>5</sub> N                 | O <sub>2</sub>         | 0.79              |                | CP/Oc-14       | $A = H_2NCSNH_2$ ; $\lambda_{\text{exc}} = 405 \text{ nm}$ . Assumed $f_r^A = 2$ .   | 737347<br>74E522 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>       | 0.92              |                | PL/LI-56       | $S' = \text{PdMPDME}$ ; rel. to $\phi_{\Delta}(S') = 1.0$ .  | 89A504<br>87E667 |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | 1.1 × 10 <sup>-3</sup> | 0.93              |                | PL/LI-56       | $S' = \text{PdTPP}$ ; rel. to $\phi_{\Delta}(S') = 1.0$ .  | 87E941           |
|  | C <sub>6</sub> H <sub>6</sub>                   | 0.1 × 10 <sup>-3</sup> | 0.57 <sup>T</sup> | 0.65           | PL/LI-56,42    | $S' = \text{Pz}$ ; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{\text{exc}} = 532 \text{ nm}$ ; used $\phi_T(S) = 0.87$ .<br>$P_T^{O_2} = 1$ .                           | 90A328           |
|  | C <sub>6</sub> H <sub>6</sub>                   | air                    | 0.78              |                | PL/LI-56,38    | $S' = \text{Pz}$ ; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{\text{exc}} = 532 \text{ nm}$ . $P_T^{O_2} = 1$ .  | 90A328           |
|  | C <sub>6</sub> H <sub>6</sub>                   | air                    | 0.68              |                | PL/LI-56       | $S' = \text{Pz}$ ; rel. to $\phi_{\Delta}(S') = 0.83$ . $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ .  | 90A328           |
|  | C <sub>6</sub> H <sub>6</sub>                   | air                    | 0.73              |                | PL/Hp-52       | $\lambda_{\text{exc}} = 560 \text{ nm}$ .  | 85E591           |
|  | C <sub>6</sub> H <sub>6</sub>                   | O <sub>2</sub>         | 0.75              |                | PL/LI-56       | $S' = \text{Pz}$ ; rel. to $\phi_{\Delta}(S') = 0.83$ . $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ .  | 90A328           |
|  | CCl <sub>4</sub>                                | air                    | 0.50              |                | MP/LI-56       | $S' = \text{Ph a}$ ; rel. to $\phi_{\Delta}(S') = 0.8$ . $P_T^{O_2} = 1$ .   | 82F161           |
| <b>2.147 Porphine, 5,10,15,20-tetrapropyl-</b>   |   |                        |                   |                |                |  |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>       | 0.74              |                | PL/LI-56       | $S' = \text{PdMPDME}$ ; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{\text{exc}} = 347 \text{ nm}$ . $P_T^{O_2} = 1$ .  | 90E615           |
| <b>2.148 Porphine, 5,10,15-tris(4-N-methylpyridyl)-20-[2-[N-[20-[5,10,15-tris(4-N-methylpyridylporphinyll-3-phenoxypropyl]-4-carboxamidobutyl]phenyl]-</b> |   |                        |                   |                |                |  |                  |
|  | H <sub>2</sub> O pH = 7                         | air                    | 0.69              |                | CP/Oc or Pa-43 | $S' = H_2\text{TMpyP}^{4+}$ ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{\text{exc}} = 436$ or 546 nm. A = Im or FFA, assumed $P_T^{O_2} = 1$ .                        | 86R162           |
| <b>2.149 Porphine-5-carboxaldehyde, 21,23-dideuterio-2,3,7,8,12,13,17,18-octaethyl-</b>  |   |                        |                   |                |                |  |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>       | 0.63              |                | PL/LI-56       | $S' = \text{PdMPDME}$ ; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{\text{exc}} = 347 \text{ nm}$ . $P_T^{O_2} = 1$ .  | 90E615           |
| <b>2.150 Porphine-5-carboxaldehyde, 2,3,7,8,12,13,17,18-octaethyl-</b>   |   |                        |                   |                |                |  |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>       | 0.63              |                | PL/LI-56       | $S' = \text{PdMPDME}$ ; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{\text{exc}} = 347 \text{ nm}$ . $P_T^{O_2} = 1$ .  | 90E615<br>89A504 |
| <b>2.151 Porphine-2,20-dicarboxylic acid, 18-(20-carboxyethyl)-12-ethenyl-7-ethyl-17,18-dihydro-3,8,13,17-tetramethyl-, cyclic 2,20-anhydride</b>          |   |                        |                   |                |                |  |                  |
|  | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O | 4 × 10 <sup>-3</sup>   | 0.83              |                | PL/LI-56       | $S' = \text{PdMPDME}$ ; rel. to $\phi_{\Delta}(S') = 1$ .  | 90E401           |
| <b>2.152 Porphine-2,18-dipropanoic acid, 7,12-bis[1-[(2-amino-2-carboxyethyl)thio]ethyl]-3,8,13,17-tetramethyl- (Porphyrin c)</b>                          |   |                        |                   |                |                |  |                  |
|  | H <sub>2</sub> O<br>pH = 7.5                    | O <sub>2</sub>         | 0.40              |                | CP/Oc-43       | $S' = \text{RB}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{\text{exc}} = 360, 400 \text{ nm}$ .  | 89F093           |
|  | H <sub>2</sub> O<br>pH = 7.5                    | O <sub>2</sub>         | 0.59              |                | CP/Oc-43       | $S' = \text{RB}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{\text{exc}} = 555, 580 \text{ nm}$ .<br>Meas. $\phi_{\Delta} = 0.33$ for porphyrin c aggregate. | 89F093           |
| <b>2.153 Porphine-2,18-dipropanoic acid, 7,12-bis[1-[(2-amino-2-carboxyethyl)thio]ethyl]-3,8,13,17-tetramethyl-, zinc(II)</b>                              |   |                        |                   |                |                |  |                  |
|  | H <sub>2</sub> O<br>pH = 7.5                    | O <sub>2</sub>         | 0.29              |                | CP/Oc-43       | $S' = \text{RB}$ ; A = FFA; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{\text{exc}} = 400, 575 \text{ nm}$ .  | 89F093           |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.  | Solvent          | [O <sub>2</sub> ] | φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method         | Comment   | Ref.   |
|--|------------------|-------------------|----------------|-----------------------------|----------------|---|--------|
| <b>2.154 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (Hematoporphyrin, HP)</b> |                  |                   |                |                             |                |   |        |
| D <sub>2</sub> O   | air <sup>a</sup> | 0.28              |                |                             | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 89E729 |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.77              |                |                             | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. contg. 2% Triton X-100.   | 89E729 |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.35              |                |                             | PL/LI-56,42    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to φ <sub>Δ</sub> (S') = 0.67; meas. φ <sub>T</sub> (S) = 0.71; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.49 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.  | 87R188 |
| D <sub>2</sub> O (mic)   | O <sub>2</sub>   |                   |                |                             | PL/LI-56,42    | S' = HP; meas. φ <sub>Δ</sub> (S)/φ <sub>Δ</sub> (S') = 2.3; λ <sub>exc</sub> = 355 nm; used φ <sub>T</sub> (S) = 0.90. Calculated f <sub>Δ</sub> <sup>T</sup> (S)/f <sub>Δ</sub> <sup>T</sup> (S') = 2.43. Soln. cont. 0.01 mol L <sup>-1</sup> CTAB; rel. to HP in D <sub>2</sub> O.  | 86E061 |
| D <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.35              |                |                             | PL/LI-56,42    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; meas. φ <sub>T</sub> (S) = 0.94; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.37 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. Soln. cont. CTAB micelles.  | 86F541 |
| D <sub>2</sub> O (mic)<br>pD = 7.4   | O <sub>2</sub>   | 0.22              | 0.32           |                             | PL/Ad-49,39    | A = DPBF; AC = S; meas. φ <sub>T</sub> (S) = 0.70; λ <sub>exc</sub> = 532 nm; used k <sub>A</sub> = 1 × 10 <sup>9</sup> L mol <sup>-1</sup> s <sup>-1</sup> . Δε <sub>T</sub> (S) = 9,770 L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm; soln. cont. 0.01 mol L <sup>-1</sup> CTAB; value questioned in [84F327].  | 83E667 |
| D <sub>2</sub> O (mic)<br>pD = 7.4   | O <sub>2</sub>   | 0.27              | 0.32           |                             | PL/Ad-49,39    | A = DPBF; AC = S; meas. φ <sub>T</sub> (S) = 0.87; λ <sub>exc</sub> = 532 nm; uscd k <sub>A</sub> = 1 × 10 <sup>9</sup> L mol <sup>-1</sup> s <sup>-1</sup> . Δε <sub>T</sub> (S) = 6,660 L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm; soln. cont. 0.07 mol L <sup>-1</sup> SDS.   | 83E667 |
| D <sub>2</sub> O/EtOH<br>(7:3)   | air <sup>a</sup> | 0.21              |                |                             | PL/LI-56       | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 337 nm. Rel. to TPP in CCl <sub>4</sub> .   | 86F316 |
| EtOH   | air <sup>a</sup> | 0.60              |                |                             | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 514.5 nm.   | 90R204 |
| EtOH   | air <sup>a</sup> | 0.67              |                |                             | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 89E729 |
| EtOH   | air              | 0.53              |                |                             | PL/Hp-52,42    | meas. φ <sub>T</sub> (S) = 0.71; λ <sub>exc</sub> = 354 nm. f <sub>Δ</sub> <sup>T</sup> = 0.75 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.  | 87E054 |
| EtOH-d <sub>1</sub>  | O <sub>2</sub>   | 0.53              |                |                             | PL/Hp-52       | λ <sub>exc</sub> = 354 nm.  | 88Z155 |
| EtOH-d <sub>6</sub>  | O <sub>2</sub>   | 0.53              |                |                             | PL/Hp-52       | λ <sub>exc</sub> = 354 nm.  | 88Z155 |
| H <sub>2</sub> O<br>pH = 7.0   | O <sub>2</sub>   | 0.48              |                |                             | CP/Pa-43       | S' = RB; A = His; rel. to φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.  | 89F580 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.08              |                |                             | CP/Pa-43       | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer; RNO as monitor for P.  | 88N170 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.37              |                |                             | CP/Oc-14       | A = Im; λ <sub>exc</sub> = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.04              |                |                             | PL/Ac-14       | A = TrpH; λ <sub>exc</sub> = 630 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.16              |                |                             | CP/Ac-14       | A = TrpH; λ <sub>exc</sub> = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
| H <sub>2</sub> O<br>pH = 7.4   | air <sup>a</sup> |                   | 0.51           |                             | PL/LI/St-55,42 | meas. φ <sub>T</sub> (S) = 0.63; λ <sub>exc</sub> = 532 nm. Δε <sub>T</sub> (S) = 4200 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; φ <sub>Δ</sub> = 0.32 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to f <sub>Δ</sub> <sup>T</sup> = 0.67 for HP in micellar soln.   | 86A407 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.45              |                |                             | CP/Ac-43       | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 546 nm. RNO as monitor of P; φ <sub>Δ</sub> = 0.36 to 0.47 at [S] = (18-160) × 10 <sup>-6</sup> , 0.35 at pH 7.0 at [S] = 3.0 × 10 <sup>-5</sup> mol L <sup>-1</sup> .  | 85R008 |
| H <sub>2</sub> O<br>pH = 7.4   | O <sub>2</sub>   | 0.41              | 0.65           |                             | PL/Ad-49,39    | A = DPBF; AC = S; λ <sub>exc</sub> = 532 nm; used k <sub>A</sub> = 1 × 10 <sup>9</sup> L mol <sup>-1</sup> s <sup>-1</sup> , φ <sub>T</sub> (S) = 0.63, ε <sub>T</sub> (AC) = 4200 L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm. Δε <sub>T</sub> (S) = 4,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm; authors suggest this supersedes f <sub>Δ</sub> <sup>T</sup> = 0.32 determined in [83E667]. | 84F327 |
| H <sub>2</sub> O pH = 7  | air              | 0.22              |                |                             | CP/Oc-43       | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = FFA; rel. to φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 546 nm.   | 84F253 |
| H <sub>2</sub> O pH = 9  | air              | 0.44              |                |                             | CP/Oc-43       | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = FFA; rel. to φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 436 nm.   | 84F253 |
| H <sub>2</sub> O pH = 7  | air              | 0.20              |                |                             | CP/Pa-43       | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; A = Im; P = Imidazole endoperoxide; rel. to φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.   | 84F253 |
| H <sub>2</sub> O (mic)   | air <sup>a</sup> | 0.53              | 0.67           |                             | PL/Ad-49,39    | A = DPBF; AC = S; meas. φ <sub>T</sub> (S) = 0.78; λ <sub>exc</sub> = 532 nm. Δε <sub>T</sub> (S) = 9,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; Soln. cont. 2% Triton X-100.   | 86A407 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]                     | $\phi_{\Delta}$ | $f_{\Delta}^T$ | Method      | Comment   | Ref.   |
|---|---|---------------------------------------|-----------------|----------------|-------------|---|--------|
| <b>2.154 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- (Hematoporphyrin, HP)—Continued</b>        |   |                                       |                 |                |             |   |        |
|   | H <sub>2</sub> O (mic)<br>pH = 7.4            | O <sub>2</sub>                        | 0.77            |                | CP/Ac-43    | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 546$ nm. Soln. cont. 0.23 mg/mL egg phosphatidylcholine; RNO as monitor of P.  | 85R008 |
|   | HCONH <sub>2</sub> /D <sub>2</sub> O<br>(9:1) | O <sub>2</sub>                        | 0.43            | 0.60           | PL/Ad-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.72$ ; $\lambda_{exc} = 532$ nm; used $k_A = 1.1 \times 10^9$ L mol <sup>-1</sup> s <sup>-1</sup> . $\Delta\varepsilon_T(S) = 10,200$ L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm.                 | 83E667 |
|   | MeOD  | O <sub>2</sub>                        | 0.64            |                | PL/Hp-52    | $\lambda_{exc} = 354$ nm.   | 88Z155 |
|   | MeOH  | air <sup>a</sup>                      | 0.52            |                | PL/LI-56    | S' = Ery; rel. to $\phi_{\Delta}(S') = 0.60$ .  | 87R138 |
|   | MeOH/D <sub>2</sub> O<br>(9:1)                | O <sub>2</sub>                        | 0.65            | 0.78           | PL/Ad-49,39 | A = DPBF; AC = S; meas. $\phi_T(S) = 0.83$ ; $\lambda_{exc} = 532$ nm; used $k_A = 1 \times 10^9$ L mol <sup>-1</sup> s <sup>-1</sup> . $\Delta\varepsilon_T(S) = 10,400$ L mol <sup>-1</sup> cm <sup>-1</sup> at 460 nm; $P_T^{O_2} = 1$ . | 83E667 |
| <b>2.155 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, cobalt(III)</b>                           |   |                                       |                 |                |             |   |        |
|   | H <sub>2</sub> O pH = 7                       | air                                   | <0.001          |                | CP/Oc-43    | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc} = 436$ or 546 nm. A = Im or FFA.  | 84F253 |
| <b>2.156 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, copper(II)</b>                            |   |                                       |                 |                |             |   |        |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0               |                | CP/Pa-43    | S' = HP; A = 2,2,6,6-Tetramethyl-4-piperidone; P = 2,2,6,6-Tetramethyl-4-piperidone N-oxyl. P monitored by esr.   | 83N270 |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0               |                | CP/Pa-43    | S' = HP; A = Im; P = Imidazole endoperoxide. Tris-buffer, RNO as monitor of P.  | 83N270 |
| <b>2.157 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, diacetate (Hematoporphyrin diacetate)</b> |   |                                       |                 |                |             |   |        |
|   | H <sub>2</sub> O<br>pH = 7.0                  | O <sub>2</sub>                        | 0.56            |                | CP/Pa-43    | S' = RB; A = His; rel. to $\phi_{\Delta}(S') = 0.75$ . RNO as monitor of P.   | 89F580 |
| <b>2.158 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, dimethyl ester (HPDME)</b>                |   |                                       |                 |                |             |   |        |
|   | C <sub>6</sub> D <sub>6</sub>                 | 1.2% O <sub>2</sub> in N <sub>2</sub> | 0.76            |                | PR/LI-60    | S' = Np; TD = BP; rel. to $f_{\Delta}^T(S') = 0.55$ . $P_T^{O_2} = 1$ ; cor. for energy transfer efficiency.  | 91A358 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.57*           |                | PL/LI-56,42 | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.72$ ; $\lambda_{exc} = 355$ nm. $f_{\Delta}^T = 0.70$ assuming $P_S^{O_2} = 0$ .   | 86E061 |
| <b>2.159 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, manganese(III)</b>                        |   |                                       |                 |                |             |   |        |
|   | H <sub>2</sub> O pH = 7                       | air                                   | <0.001          |                | CP/Oc-43    | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to $\phi_{\Delta}(S') = 0.74$ ; $\lambda_{exc} = 436$ or 546 nm. A = Im or FFA.  | 84F253 |
| <b>2.160 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, nickel(II)</b>                            |   |                                       |                 |                |             |   |        |
|   | DMF   | O <sub>2</sub>                        | 0.02            |                | CP/Pa-43    | S' = HP; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethyl-piperidine N-oxyl; rel. to $\phi_{\Delta}(S') = 0.6^b$ . Obs. P by esr  | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.02            |                | CP/Ac-43    | S' = HP; A = Pd(phen)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ . Obs. P by esr   | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.02            |                | CP/Ac-43    | S' = HP; A = Pd(bpy)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ .  | 91F203 |
| <b>2.161 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, palladium(II)</b>                         |   |                                       |                 |                |             |   |        |
|   | DMF   | O <sub>2</sub>                        | 0.39            |                | CP/Pa-43    | S' = HP; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethyl-piperidine N-oxyl; rel. to $\phi_{\Delta}(S') = 0.6^b$ . Obs. P by esr  | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.36            |                | CP/Ac-43    | S' = HP; A = Pd(phen)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ .   | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.38            |                | CP/Ac-43    | S' = HP; A = Pd(bpy)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ .  | 91F203 |
| <b>2.162 Porphine-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, platinum(II)</b>                          |   |                                       |                 |                |             |   |        |
|   | DMF   | O <sub>2</sub>                        | 0.26            |                | CP/Pa-43    | S' = HP; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethyl-piperidine N-oxyl; rel. to $\phi_{\Delta}(S') = 0.6^b$ . Obs. P by esr  | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.25            |                | CP/Ac-43    | S' = HP; A = Pd(phen)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ .   | 91F203 |
|   | DMF   | O <sub>2</sub>                        | 0.24            |                | CP/Ac-43    | S' = HP; A = Pd(bpy)(dmt); rel. to $\phi_{\Delta}(S') = 0.6^b$ .  | 91F203 |
| <b>2.163 Porphine-2,18-dipropanoic acid, 7,12-bis(2-hydroxyethyl)-3,8,13,17-tetramethyl- (Isohematoporphyrin)</b>                   |   |                                       |                 |                |             |   |        |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | air <sup>a</sup>                      | 0.66            |                | CP/Pa-43    | S' = [22]Coproporphyrin II; A = 2,5-DMF. Rel. to $\phi_{\Delta}(S') = 1.1$ , using $\phi_{\Delta}(RB) = 0.80^b$ .   | 90R215 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]   | $\phi_{\Delta}$   | $f_{\Delta}^T$  | Method   | Comment  | Ref.   |
|-------|---|---|---|---|--|--|--|
| 2.164 | Porphine-2,18-dipropanoic acid, 7,12-bis(1-methoxyethyl)-3,7,12,17-tetramethyl-, dianion                                      | D <sub>2</sub> O/EtOH<br>(7:3)  | air <sup>a</sup>  | 0.49  | PL/LI-56   | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.7$ ; $\lambda_{exc} = 337$ nm. Rel. to TPP in CCl <sub>4</sub> .  | 86F316   |
| 2.165 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- (Protoporphyrin, PP)                                    | D <sub>2</sub> O<br>D <sub>2</sub> O (mic)<br>H <sub>2</sub> O<br>pH = 8.0  | air <sup>a</sup><br>air   | ≤0.02<br>0.56<br>0.14   | PL/LI-56<br>CP/Pa-43   | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . Colloidal soln. contg. 0.5% NH <sub>4</sub> OH.<br>S' = HP; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.4^b$ . Triton X-100.  | 88F450<br>83N270   |
| 2.166 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (PPDME)                                 | C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O<br>C <sub>5</sub> H <sub>5</sub> N<br>C <sub>5</sub> H <sub>5</sub> N<br>C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub><br>C <sub>6</sub> D <sub>6</sub><br>C <sub>6</sub> H <sub>6</sub><br>CCl <sub>4</sub><br>CCl <sub>4</sub> | air <sup>a</sup><br>O <sub>2</sub><br>O <sub>2</sub><br>air <sup>a</sup><br>0.1 × 10 <sup>-3</sup><br>1.2% O <sub>2</sub> in N <sub>2</sub><br>air<br>air<br>air <sup>a</sup><br>O <sub>2</sub><br>O <sub>2</sub><br>air<br>air | 0.77<br>0.70<br>1.1<br>0.80<br>0.45 <sup>T</sup><br>0.79<br>0.73<br>0.59<br>0.65*<br>0.57<br>0.63<br>0.57<br>0.70<br>0.77 | PL/LI-56<br>CP/Oc-14<br>CP/Oc-14<br>PL/LI-56<br>PL/LI-56,42<br>PR/LI-60<br>PL/LI-56,38<br>PL/LI-56<br>PL/LI-56,42<br>PL/LI-56<br>PL/LI-56,42<br>PL/LI-56<br>MP/LI-56<br>MP/LI-56 | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ .<br>A = H <sub>2</sub> NCSNH <sub>2</sub> . Assumed $f_t^A = 2$ .<br>A = Pregnolone.<br>S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ .<br>S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 532$ nm; used $\phi_T(S) = 0.66$ . $P_T^{O_2} = 1$ .<br>S' = Np; TD = BP; rel. to $f_{\Delta}^T(S') = 0.55$ . $P_T^{O_2} = 1$ ; cor. for energy transfer efficiency.<br>S' = Pz; rel. to $f_{\Delta}^T(S') = 1.0$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$ .<br>S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ .<br>S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.66$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.86$ assuming $P_S^{O_2} = 0$ ; used $P_T^{O_2} = 1$ .<br>S' = Pz; rel. to $\phi_{\Delta}(S') = 0.83$ ; $\lambda_{exc} = 532$ nm. $P_T^{O_2} = 1$ ; assumed $f_T^{O_2} = 1$ .<br>S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; $\lambda_{exc} = 347$ nm; used $\phi_T(S) = 0.80$ . $f_{\Delta}^T = 0.71$ assuming $P_S^{O_2} = 0$ ; used $P_T^{O_2} = 1$ .<br>S' = Ph a; rel. to $\phi_{\Delta}(S') = 0.8$ . $P_T^{O_2} = 1$ .<br>S' = Chl a; rel. to $\phi_{\Delta}(S') = 0.55$ . $P_T^{O_2} = 1$ . | 88F450<br>74E522<br>587002<br>90E615<br>90A328<br>90A328<br>90A328<br>90A328<br>87R185<br>90A328<br>90A328<br>87R185<br>86E061<br>82F161<br>80E714<br>79A010 |
| 2.167 | Porphine-2,18-dipropanoic acid, 21,23-dideutero-7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester (PPDME-d <sub>2</sub> ) | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | air <sup>a</sup>  | 0.80  | PL/LI-56   | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ .  | 90E615   |
| 2.168 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester, magnesium(II)                          | (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O   | air <sup>a</sup>  | 0.77  | PL/LI-56   | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.70$ .   | 88F450   |
| 2.169 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester, zinc(II)                               | CCl <sub>4</sub>  | air   | 0.65  | MP/LI-56   | S' = Ph a; rel. to $\phi_{\Delta}(S') = 0.8$ .   | 82F161   |
| 2.170 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, magnesium(II) (MgPP)                                   | D <sub>2</sub> O<br>D <sub>2</sub> O (mic)  | air <sup>a</sup><br>air <sup>a</sup>  | ≤0.02<br>0.56   | PL/LI-56<br>PL/LI-56   | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . Colloidal soln. contg. 0.5% NH <sub>4</sub> OH.<br>S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.70$ . Soln. cont. 1% Triton X-100.  | 88F450<br>88F450   |
| 2.171 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester, palladium(II) (PdPPDME)                | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>   | 1.8 × 10 <sup>-3</sup>  | 0.95  | PL/LI-56   | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ ; $\lambda_{exc} = 347$ nm.  | 87E667   |
| 2.172 | Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dichlorotin(IV)  | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.33  | PL/LI-56,42  | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; meas. $\phi_T(S) = 0.68$ ; $\lambda_{exc} = 347$ nm. $f_{\Delta}^T = 0.48$ assuming $P_S^{O_2} = 0$ ; soln. cont. CTAB micelles.  | 86F541   |

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ]                     | Φ <sub>Δ</sub> | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment   | Ref.             |
|--|---|---------------------------------------|----------------|-----------------------------|-------------|---|------------------|
| <b>2.172 Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dichlorotin(IV)—Continued</b>                                  |   |                                       |                |                             |             |   |                  |
|  | MeOD  | O <sub>2</sub>                        | 0.70*          |                             | PL/LI-56    | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; λ <sub>exc</sub> = 347 nm. Recalcd. using Φ <sub>Δ</sub> (S') = 0.64 from [88Z155]; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 88R194           |
| <b>2.173 Porphine-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, zinc(II) (ZnPP)</b>  |   |                                       |                |                             |             |   |                  |
|  | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.05           |                             | CP/Pa-43    | S' = HP; A = 2,2,6,6-Tetramethyl-4-piperidone; P = 2,2,6,6-Tetramethyl-4-piperidone N-oxyl; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> . P monitored by esr.  | 83N270           |
|  | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.04           |                             | CP/Pa-43    | S' = HP; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> . Tris-buffer, RNO as monitor of P.   | 83N270           |
| <b>2.174 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl] ester</b> |   |                                       |                |                             |             |   |                  |
|  | CH <sub>2</sub> Cl <sub>2</sub>               | air                                   | 0.22           |                             | PL/LI-56    | S' = MPDME; rel. to Φ <sub>Δ</sub> (S') = 0.65*; 0.57; λ <sub>exc</sub> = 532 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in benzene.   | 91E134           |
|  | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>                        | 0.16           |                             | CP/Ac-43    | S' = MPDME; A = BRH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.57.  | 89F267           |
| <b>2.175 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, di[4-(diphenylmethylaminocarbonylphenylmethyl] ester</b>         |   |                                       |                |                             |             |   |                  |
|  | CH <sub>2</sub> Cl <sub>2</sub>               | air                                   | 0.57           |                             | PL/LI-56    | S' = MPDME; rel. to Φ <sub>Δ</sub> (S') = 0.57; λ <sub>exc</sub> = 532 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in benzene.  | 91E134           |
|  | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>                        | 0.54           |                             | CP/Ac-43    | S' = MPDME; A = BRH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.57.  | 89F267           |
| <b>2.176 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, diethyl ester (MPDEE)</b>  |   |                                       |                |                             |             |   |                  |
|  | C <sub>5</sub> H <sub>5</sub> N               | O <sub>2</sub>                        | 0.70           |                             | CP/Oc-14    | A = H <sub>2</sub> NCSNH <sub>2</sub> ; λ <sub>exc</sub> = 430 nm. Assumed f <sub>r</sub> <sup>A</sup> = 2.   | 737347<br>74E522 |
| <b>2.177 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester (MPDME)</b>                                       |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 0.73           |                             | PL/LI-56,42 | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E543<br>87E667 |
|  | C <sub>6</sub> D <sub>6</sub>                 | 1.2% O <sub>2</sub> in N <sub>2</sub> |                | 0.88                        | PR/LI-60    | S' = Np; TD = BP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for energy transfer efficiency.  | 91A358           |
|  | C <sub>6</sub> D <sub>6</sub>                 | air <sup>a</sup>                      | 0.61           |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; meas. Φ <sub>T</sub> (S) = 0.81; λ <sub>exc</sub> = 347 nm. f <sub>Δ</sub> <sup>T</sup> = 0.73 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. | 87R185           |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.65*          |                             | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 347 nm; used Φ <sub>T</sub> (S) = 0.81. f <sub>Δ</sub> <sup>T</sup> = 0.71 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; used P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 87R185<br>86E061 |
|  | CCl <sub>4</sub>                              | air                                   | 0.90           |                             | MP/LI-56    | S' = Ph a; rel. to Φ <sub>Δ</sub> (S') = 0.8. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F161           |
|  | CH <sub>3</sub> CN                            | air <sup>a</sup>                      | 0.61           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E543           |
| <b>2.178 Porphine-2,18-dipropanoic acid, 21,23-dideutero-7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester (MPDME-d<sub>2</sub>)</b>         |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 0.73           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 90E615           |
| <b>2.179 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, cadmium(II)</b>                                  |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup>                | 0.76           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E667           |
| <b>2.180 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, copper(II)</b>                                   |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | ~0.5           |                             | PL/LI-56    | S' = PdOEP; rel. to Φ <sub>Δ</sub> (S') = 1 <sup>b</sup> ; λ <sub>exc</sub> = 347 nm.   | 91E392           |
|  | CCl <sub>4</sub>                              | air <sup>a</sup>                      |                |                             | PL/LI-56    | S' = GaTPP; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.62; λ <sub>exc</sub> = 347 nm.   | 91E392           |
| <b>2.181 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, magnesium(II)</b>                                |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 0.56           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E543<br>87E667 |
|  | CH <sub>3</sub> CN                            | air <sup>a</sup>                      | 0.56           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 347 nm.   | 87E543           |
| <b>2.182 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, mercury(II)</b>                                  |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup>                | 0.58           |                             | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.   | 87E667           |
| <b>2.183 Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, palladium(II)</b>                                |   |                                       |                |                             |             |   |                  |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 1.0            |                             |             | Reference value justified in [74E522] and [78E893].   | 82E010           |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]                             | Φ <sub>Δ</sub>             | f <sub>Δ</sub> <sup>T</sup> | Method      | Comment  | Ref.  |        |
|-------|--|---|----------------------------|-----------------------------|-------------|--|---|--------|
| 2.184 | Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, oxovanadium(IV)                                       | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup>     | 0.96                        | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.  | 87E667  |        |
| 2.185 | Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, zinc(II)  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | 1.8 × 10 <sup>-3</sup>     | 0.82                        | PL/LI-56    | S' = PdMPDME; rel. to Φ <sub>Δ</sub> (S') = 1.0; λ <sub>exc</sub> = 347 nm.  | 87E667  |        |
| 2.186 | Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, [4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl] methyl ester     | CH <sub>2</sub> Cl <sub>2</sub>               | air                        | 0.40                        | PL/LI-56    | S' = MPDME; rel. to Φ <sub>Δ</sub> (S') = 0.57; λ <sub>exc</sub> = 532 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in benzene.   | 91E134  |        |
| 2.187 | Porphine-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, mono[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl] ester        | CH <sub>2</sub> Cl <sub>2</sub>               | air                        | 0.37                        | PL/LI-56    | S' = MPDME; rel. to Φ <sub>Δ</sub> (S') = 0.57; λ <sub>exc</sub> = 532 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; rel. to S' in benzene.   | 91E134  |        |
| 2.188 | Porphine-2,18-dipropanoic acid, 7,12-diformyl-1-3,8,13,17-tetramethyl-, dimethyl ester   | CH <sub>2</sub> Cl <sub>2</sub>               | air <sup>a</sup>           | 0.68                        | CP/Ac-43    | S' = PPDME; A = DPF; rel. to Φ <sub>Δ</sub> (S') = 0.77; λ <sub>exc</sub> = 405-408 nm.  | 82F333  |        |
| 2.189 | Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-ethyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, (Z)            | CHCl <sub>3</sub>                             | air                        | 0.62 <sup>T</sup>           | 0.9         | CP/Ac-14,42  | A = MDH; meas. Φ <sub>T</sub> (S) = 0.69; λ <sub>exc</sub> = 405, 660 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. Used f <sub>r</sub> <sup>A</sup> = 0.30, cor. for quenching of fluorescence of S.  | 90R006 |
|       |  | CHCl <sub>3</sub>                             | air                        | 0.54 <sup>T</sup>           | 0.8         | CP/LI-56,42  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.50; meas. Φ <sub>T</sub> (S) = 0.69; λ <sub>exc</sub> = 405 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. Same value in O <sub>2</sub> , cor. for quenching of fluorescence of S and S'.               | 90R006 |
| 2.190 | Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-ethylidene-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester,           | CCl <sub>4</sub>                              | air                        | 0.58                        | CP/Ac-14    | A = MDH. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used f <sub>r</sub> <sup>A</sup> = 0.30.   | 90R006  |        |
|       |  | CHCl <sub>3</sub>                             | (1.2-9) × 10 <sup>-3</sup> | 0.95                        | CP/Ac-14,39 | A = MDH; meas. Φ <sub>T</sub> (S) = 0.57. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; used f <sub>r</sub> <sup>A</sup> = 0.30; measured f <sub>Δ</sub> <sup>T</sup> Φ <sub>T</sub> = 0.54, f <sub>Δ</sub> <sup>T</sup> f <sub>T</sub> <sup>O<sub>2</sub></sup> = 0.87; cor. for quenching of fluorescence of S. | 90R006  |        |
|       |  | CHCl <sub>3</sub>                             | air                        | 0.54 <sup>T</sup>           | 0.95        | CP/LI-56,42  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.50; meas. Φ <sub>T</sub> (S) = 0.57; λ <sub>exc</sub> = 405 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1. cor. for quenching of fluorescence of S and S'.  | 90R006 |
| 2.191 | Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, (Z)           | CHCl <sub>3</sub>                             | air <sup>a</sup>           | 0.60                        | 0.85        | CP/LI-56,42  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.5; meas. Φ <sub>T</sub> (S) = 0.71; λ <sub>exc</sub> = 405 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 91R253 |
| 2.192 | Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, tin(IV), (Z)  | CHCl <sub>3</sub>                             | air <sup>a</sup>           | 0.62                        | 0.65        | CP/LI-56,42  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.5; meas. Φ <sub>T</sub> (S) = 0.95; λ <sub>exc</sub> = 405 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 91R253 |
| 2.193 | Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, zinc(II), (Z) | CHCl <sub>3</sub>                             | air <sup>a</sup>           | 0.61                        | 0.69        | CP/LI-56,42  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.5; meas. Φ <sub>T</sub> (S) = 0.88; λ <sub>exc</sub> = 405 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 91R253 |
| 2.194 | Porphine-2,18-dipropanoic acid, 7(12)-ethenyl-12(7)-formyl, dimethyl ester   | CH <sub>2</sub> Cl <sub>2</sub>               | air <sup>a</sup>           | 0.71                        | CP/Ac-43    | S' = PPDME; A = DPF; rel. to Φ <sub>Δ</sub> (S') = 0.77; λ <sub>exc</sub> = 405-408 nm.  | 82F333  |        |
| 2.195 | Porphine-2,18-dipropanoic acid, 7-ethenyl-12-(1-hydroxyethyl)-3,8,13,17-tetramethyl-   | EtOD  | air                        | 0.45                        | 0.65        | PL/LI-56,42  | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.53; meas. Φ <sub>T</sub> (S) = 0.69; λ <sub>exc</sub> = 347 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 87E054 |
|       |  | D <sub>2</sub> O                              | O <sub>2</sub>             | 0.2                         |             | PL/LI-56,42  | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> ; meas. Φ <sub>T</sub> (S) = 0.34; λ <sub>exc</sub> = 355 nm. Calculated f <sub>Δ</sub> <sup>T</sup> (S)f <sub>Δ</sub> <sup>T</sup> (S') = 1.19.  | 86E061 |
|       |  | D <sub>2</sub> O (mic)                        | O <sub>2</sub>             | 0.6                         |             | PL/LI-56,42  | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> ; meas. Φ <sub>T</sub> (S) = 0.63; λ <sub>exc</sub> = 355 nm. Calculated f <sub>Δ</sub> <sup>T</sup> (S)f <sub>Δ</sub> <sup>T</sup> (S') = 2.25; soln. cont. 0.01 mol L <sup>-1</sup> CTAB. | 86E061 |
| 2.196 | Porphine-2,18-dipropanoic acid, 12(7)-ethenyl-8(13)-hydroxy-3,8,13,17-tetramethyl-7(12)-(oxoethylidene)-, dimethyl ester                   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>             | 0.56*                       | PL/LI-56,42 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 355 nm; used Φ <sub>T</sub> (S) = 0.66. f <sub>Δ</sub> <sup>T</sup> = 0.74 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.   | 86E061  |        |
|       |  | CH <sub>2</sub> Cl <sub>2</sub>               | air <sup>a</sup>           | 0.49                        |             |  |   |        |
|       |  |   |                            | 0.69                        | CP/Ac-43    | S' = PPDME; A = DPF; rel. to Φ <sub>Δ</sub> (S') = 0.77; λ <sub>exc</sub> = 405-408 nm.  | 82F333  |        |

Table 2. Quantum yields of photosensitized production of singlet oxygen, porphyrins.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ]                     | $\phi_{\Delta}$ | $f_{\Delta}^T$ | Method  | Comment | Ref.   |
|---|---|---------------------------------------|-----------------|----------------|---|---------|--------|
| <b>2.197 Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- (Deuteroporphyrin, DP)</b>  |   |                                       |                 |                |   |         |        |
|   | H <sub>2</sub> O<br>pH = 7.0                  | O <sub>2</sub>                        | 0.51            | CP/Pa-43       | S' = RB; A = His; rel. to $\phi_{\Delta}(S') = 0.75$ . RNO as monitor of P.   |         | 89F580 |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.22            | CP/Pa-43       | S' = HP; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.4^b$ . Tris-buffer, RNO as monitor of P.  |         | 83N270 |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.23            | CP/Pa-43       | S' = HP; A = 2,2,6,6-Tetramethyl-4-piperidone; P = 2,2,6,6-Tetramethyl-4-piperidone N-oxyl; rel. to $\phi_{\Delta}(S') = 0.4^b$ . P monitored by esr.   |         | 83N270 |
| <b>2.198 Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl-, dimethyl ester (DPDME)</b>   |   |                                       |                 |                |   |         |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 0.53            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1.0$ .   |         | 89A504 |
|   | C <sub>6</sub> D <sub>6</sub>                 | 1.2% O <sub>2</sub> in N <sub>2</sub> | 0.75            | PR/LI-60       | S' = Np; TD = BP; rel. to $f_{\Delta}^T(S') = 0.55$ . $P_T^{O_2} = 1$ ; cor. for energy transfer efficiency.  |         | 91A358 |
|   | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.64*           | PL/LI-56,42    | S' = Ac; rel. to $\phi_{\Delta}(S') = 0.73$ ; meas. $\phi_T(S) = 0.72$ ; $\lambda_{exc} = 355$ nm.<br>$f_{\Delta}^T = 0.78$ assuming $P_S^{O_2} = 0$ .  |         | 86E061 |
|   |   |                                       | 0.56            |                |   |         |        |
| <b>2.199 Porphine-2,18-dipropanoic acid, 21,23-dideutero-3,7,12,17-tetramethyl-, dimethyl ester (DPDME-d<sub>2</sub>)</b>                           |   |                                       |                 |                |   |         |        |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>                      | 0.58            | PL/LI-56       | S' = PdMPDME; rel. to $\phi_{\Delta}(S') = 1$ ; $\lambda_{exc} = 347$ nm. $P_T^{O_2} = 1$ .   |         | 90E615 |
| <b>2.200 Porphine-2-propanoic acid, 18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12,17-tetramethyl- (Chlorin a<sub>6</sub>)</b> |   |                                       |                 |                |   |         |        |
|   | C <sub>5</sub> H <sub>5</sub> N               | air <sup>a</sup>                      | 0.74            | PL/LI-56       | S' = TPP; rel. to $\phi_{\Delta}(S') = 0.74$ ; meas. $\phi_T(S) = 0.81$ ; $\lambda_{exc} = 347$ nm.   |         | 89E505 |
|   | D <sub>2</sub> O<br>pD = 8.1                  | air <sup>a</sup>                      | 0.75            | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.7$ ; meas. $\phi_T(S) = 0.82$ ; $\lambda_{exc} = 347$ nm. Complex with HSA.   |         | 89E505 |
|   | D <sub>2</sub> O<br>pD = 8.1                  | air <sup>a</sup>                      | 0.76            | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.7$ ; meas. $\phi_T(S) = 0.80$ ; $\lambda_{exc} = 347$ nm.   |         | 89E505 |
|   | D <sub>2</sub> O (mic)<br>pD = 8.1            | air <sup>a</sup>                      | 0.70            | PL/LI-56       | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to $\phi_{\Delta}(S') = 0.7$ ; meas. $\phi_T(S) = 0.80$ ; $\lambda_{exc} = 347$ nm. Soln. cont. 10 <sup>-3</sup> mol L <sup>-1</sup> Triton X-100.  |         | 89E505 |
| <b>2.201 5-Porphinepropenoic acid, octaethyl-, ethyl ester</b>  |   |                                       |                 |                |   |         |        |
|   | MeOH  | air                                   | 0.08            | PL/LI-56,42    | S' = HP; rel. to $\phi_{\Delta}(S') = 0.64$ ; meas. $\phi_T(S) = 0.08$ . $f_{\Delta}^T = \sim 1$ assuming $P_S^{O_2} = 0$ ; $P_T^{O_2} = 1$ ; secondary $\phi_{\Delta}(S') = 0.41$ , S' = ZnPCS.  |         | 90E491 |
| <b>2.202 Porphine-2-propionamide, N-[4-[(7-chloro-4-quinolyl)amino]butyl]-5,10,15,20-tetraphenyl-</b>   |   |                                       |                 |                |   |         |        |
|   | H <sub>2</sub> O (mic)                        | air                                   |                 | CP/Ac-43       | S' = HP; A = His; meas. $\phi_{\Delta}(S)/\phi_{\Delta}(S') = 0.65$ ; $\lambda_{exc} = 405$ nm. Tris buffer, 1% Triton X-100.   |         | 90F450 |
| <b>2.203 Porphine-2,7,12,17-tetrapropanoic acid, 3,8,13,18-tetrakis(carboxymethyl)- (Uroporphyrin I)</b>  |   |                                       |                 |                |   |         |        |
|   | H <sub>2</sub> O<br>pH = 7.4                  | air <sup>a</sup>                      | 0.56            | PL/LI,St-55,42 | S' = HP; rel. to $f_{\Delta}^T(S') = 0.51$ ; mcas. $\phi_T(S) = 0.93$ ; $\lambda_{exc} = 532$ nm; used $\epsilon_T(S) = 19000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm. $\Delta\epsilon_T(S) = 19,000$ L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; $\phi_{\Delta} = 0.52$ assuming $P_S^{O_2} = 0$ ; $P_T^{O_2} = 1$ . |         | 86A407 |
|   | H <sub>2</sub> O<br>pH = 7.4                  | O <sub>2</sub>                        | 0.71            | CP/Ac-43       | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 546$ nm. RNO as monitor of P.  |         | 85R008 |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.80            | CP/Pa-43       | S' = HP; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.4^b$ . Tris-buffer, RNO as monitor of P.  |         | 83N270 |
|   | H <sub>2</sub> O<br>pH = 8.0                  | air                                   | 0.62            | CP/Pa-43       | S' = HP; A = 2,2,6,6-Tetramethyl-4-piperidone; P = 2,2,6,6-Tetramethyl-4-piperidone N-oxyl; rel. to $\phi_{\Delta}(S') = 0.4^b$ . P monitored by esr.   |         | 83N270 |
|   | H <sub>2</sub> O (mic)<br>pH = 7.4            | O <sub>2</sub>                        | 0.92            | CP/Ac-43       | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to $\phi_{\Delta}(S') = 0.75$ ; $\lambda_{exc} = 546$ nm. Soln. cont. 0.23 mg/mL egg phosphatidylcholine; RNO as monitor of P.  |         | 85R008 |
| <b>2.204 Porphine-2,7,12,17-tetrapropanoic acid, 3,8,13,18-tetramethyl- (Coproporphyrin I)</b>  |   |                                       |                 |                |   |         |        |
|   | H <sub>2</sub> O<br>pH = 7.0                  | O <sub>2</sub>                        | 0.60            | CP/Pa-43       | S' = RB; A = His; rel. to $\phi_{\Delta}(S') = 0.75$ . RNO as monitor of P.   |         | 89F580 |
| <b>2.205 Porphine-2,7,12,18-tetrapropanoic acid, 3,8,13,17-tetramethyl- (Coproporphyrin III)</b>  |   |                                       |                 |                |   |         |        |
|   | H <sub>2</sub> O<br>pH = 7.4                  | air <sup>a</sup>                      | 0.46            | PL/LI,St-55,42 | S' = HP; rel. to $f_{\Delta}^T(S') = 0.51$ ; meas. $\phi_T(S) = 0.61$ ; $\lambda_{exc} = 532$ nm. $\Delta\epsilon_T(S) = 6500$ L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; $\phi_{\Delta} = 0.28$ assuming $P_S^{O_2} = 0$ ; $P_T^{O_2} = 1$ .  |         | 86A407 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ]                     | Φ <sub>Δ</sub>    | f <sub>Δ</sub> <sup>T</sup> | Method   | Comment | Ref.   |
|--|---|---------------------------------------|-------------------|-----------------------------|--|---------|--------|
| <b>2.205 Porphine-2,7,12,18-tetrapropionic acid, 3,8,13,17-tetramethyl- (Coproporphyrin III)—Continued</b> |   |                                       |                   |                             |  |         |        |
|  | H <sub>2</sub> O (mic)                        | air <sup>a</sup>                      | 0.71              | PL/LI-St-55,42              | S' = HP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.67; meas. Φ <sub>T</sub> (S) = 0.81; λ <sub>exc</sub> = 532 nm. Δε <sub>T</sub> (S) = 12,200 L mol <sup>-1</sup> cm <sup>-1</sup> at 440 nm; Φ <sub>Δ</sub> = 0.58 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; Soln. cont. 2% Triton X-100. |         | 86A407 |
| <b>2.206 Porphine-2,7,12,18-tetrapropionic acid, 3,8,13,17-tetramethyl-, tetramethyl ester</b>             |   |                                       |                   |                             |  |         |        |
|  | C <sub>6</sub> D <sub>6</sub>                 | 1.2% O <sub>2</sub> in N <sub>2</sub> | 0.74              | PR/LI-60                    | S' = Np; TD = BP; rel. to f <sub>Δ</sub> <sup>T</sup> (S') = 0.55. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; cor. for energy transfer efficiency.   |         | 91A358 |
| <b>2.207 Porphine-2,7,18-tripropionic acid, 13,13'-(1,6-hexanediyil)bis[3,8,12,17-tetramethyl-</b>         |   |                                       |                   |                             |  |         |        |
|  | D <sub>2</sub> O (mic)                        | O <sub>2</sub>                        | 0.18              | PL/LI-56                    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 355 nm. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.   |         | 88R204 |
| <b>2.208 Porphine-2,7,18-tripropionic acid, 13,13'-(1,3-propanediyil)bis[3,8,12,17-tetramethyl-</b>        |   |                                       |                   |                             |  |         |        |
|  | D <sub>2</sub> O (mic)                        | O <sub>2</sub>                        | 0.18              | PL/LI-56                    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 355 nm. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.   |         | 88R204 |
| <b>2.209 Porphine-2,7,18-tripropionic acid, 13,13'-(1,11-undecanediyil)bis[3,8,12,17-tetramethyl-</b>      |   |                                       |                   |                             |  |         |        |
|  | D <sub>2</sub> O (mic)                        | O <sub>2</sub>                        | 0.18              | PL/LI-56                    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 355 nm. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.   |         | 88R204 |
| <b>2.210 [26] Porphyrin</b>  |   |                                       |                   |                             |  |         |        |
|  | CHCl <sub>3</sub>                             | air                                   | 0.14 <sup>T</sup> | PL/LI-56,42                 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.50; meas. Φ <sub>T</sub> (S) = 0.15; λ <sub>exc</sub> = 546 nm. f <sub>Δ</sub> <sup>T</sup> = -1 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  |         | 90E530 |
| <b>2.211 Porphycene</b>  |   |                                       |                   |                             |  |         |        |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air                                   | 0.30              | PL/LI-56,42                 | S' = An; rel. to Φ <sub>Δ</sub> (S') = 0.61; meas. Φ <sub>T</sub> (S) = 0.42; λ <sub>exc</sub> = 347 and 354 nm. Assumed P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0 and P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 to give f <sub>Δ</sub> <sup>T</sup> = 0.7.  |         | 86E633 |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.34              | PL/LI-56                    | S' = ZnTPP; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 600 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  |         | 90E374 |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.34              | PL/LI-56,42                 | S' = An; rel. to Φ <sub>Δ</sub> (S') = 0.68; meas. Φ <sub>T</sub> (S) = 0.3; λ <sub>exc</sub> = 354 nm. Assumed P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0 and P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 to give f <sub>Δ</sub> <sup>T</sup> = 1.   |         | 90E374 |
|  | D <sub>2</sub> O (ves)<br>pD = 7.4            | O <sub>2</sub>                        | 0.17-<br>0.37     | PL/LI-56                    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.72; λ <sub>exc</sub> = 600 nm. [DPPC] = 6.7 × 10 <sup>-4</sup> mol L <sup>-1</sup> , S' in D <sub>2</sub> O-Tris buffer; concn. dependent.  |         | 90N126 |
|  | EtOH  | air                                   | 0.30              | PL/LI-56                    | S' = An; rel. to Φ <sub>Δ</sub> (S') = 0.61; λ <sub>exc</sub> = 347 and 354 nm. Also relative to Φ <sub>Δ</sub> = 0.73 for ZnTPP.  |         | 86E633 |
| <b>2.212 Porphycene, 2,7,12,17-tetrapropyl-</b>  |   |                                       |                   |                             |  |         |        |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air                                   | 0.35              | PL/LI-56                    | S' = An; rel. to Φ <sub>Δ</sub> (S') = 0.61; λ <sub>exc</sub> = 347 and 354 nm. Also relative to Φ <sub>Δ</sub> = 0.73 for ZnTPP; some singlet quenching.  |         | 86E633 |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.36              | PL/LI-56                    | S' = ZnTPP; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 600 nm.   |         | 90E374 |
|  | C <sub>6</sub> H <sub>6</sub>                 | O <sub>2</sub>                        | 0.36              | PL/LI-56,42                 | S' = An; rel. to Φ <sub>Δ</sub> (S') = 0.68; meas. Φ <sub>T</sub> (S) = 0.4; λ <sub>exc</sub> = 354 nm. Measured P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0 and P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1 to give f <sub>Δ</sub> <sup>T</sup> = 1.  |         | 90E374 |
|  | D <sub>2</sub> O (ves)<br>pD = 7.4            | O <sub>2</sub>                        | 0.22-<br>0.37     | PL/LI-56                    | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.72; λ <sub>exc</sub> = 553 nm. [DPPC] = 6.7 × 10 <sup>-4</sup> mol L <sup>-1</sup> , S' in D <sub>2</sub> O-Tris buffer; concn. dependent.  |         | 90N126 |
| <b>2.213 Sapphyrin, 3,8,12,13,17,22-hexaethyl-2,7,18,23-tetramethyl-, diprotonated</b>                     |   |                                       |                   |                             |  |         |        |
|  | CD <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>                        | 0.28              | PL/LI-56,41                 | S' = RBEE; rel. to Φ <sub>Δ</sub> (S') = 0.61; λ <sub>exc</sub> = 355, 532 nm. f <sub>Δ</sub> <sup>T</sup> = -0.5 assuming P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0; SAP <sup>2+</sup> exists as monomer in CHCl <sub>3</sub> where Φ <sub>T</sub> (S) = 0.54.  |         | 90E194 |
|  | CD <sub>3</sub> CN                            | O <sub>2</sub>                        | 0.19              | PL/LI-56                    | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.37; λ <sub>exc</sub> = 355 nm. SAP <sup>2+</sup> exists as mixt. of monomer and dimer in this solvent; at high concn. of SAP <sup>2+</sup> (1 × 10 <sup>-4</sup> mol L <sup>-1</sup> ), Φ <sub>Δ</sub> = 0.17.  |         | 90E194 |
|  | CD <sub>3</sub> OD                            | air                                   | 0.13              | PL/LI-56                    | S' = T(m-HOP)P; rel. to Φ <sub>Δ</sub> (S') = 0.57; λ <sub>exc</sub> = 355, 532 nm. SAP <sup>2+</sup> exists as mixt. of monomer and dimer in this solvent.  |         | 90E194 |
| <b>2.214 Tetrabenzoporphine, zinc(II)</b>  |   |                                       |                   |                             |  |         |        |
|  | C <sub>5</sub> H <sub>4</sub> N/diox<br>(1:1) | O <sub>2</sub>                        | 0.7               | PL/LI-56                    | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.6 <sup>b</sup> ; λ <sub>exc</sub> = 633 nm.   |         | 91F205 |

Table 2. Quantum yields of photosensitized production of singlet oxygen, from porphyrins and related species.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]                             | $\phi_{\Delta}$  | $f_{\Delta}^T$ | Method   | Comment   | Ref.  |        |
|-------|---|---|------------------|----------------|----------|---|---|--------|
| 2.215 | Tetrabenz[b,g,l,q]porphine, 6,13-diphenyl-, cadmium(II)   | diox  | O <sub>2</sub>   | 0.5            | PL/LI-56 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.6^b$ ; $\lambda_{exc} = 633$ nm. | 91F205  |        |
| 2.216 | Tetrabenz[b,g,l,q]porphine, 6,13-diphenyl-, magnesium(II) | diox  | O <sub>2</sub>   | 0.4            | PL/LI-56 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.6^b$ ; $\lambda_{exc} = 633$ nm. | 91F205  |        |
| 2.217 | Tetrabenz[b,g,l,q]porphine, 6,13-diphenyl-, zinc(II)      | C <sub>6</sub> H <sub>5</sub> N/diox<br>(1:1) | O <sub>2</sub>   | 0.6            | PL/LI-56 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.6^b$ ; $\lambda_{exc} = 633$ nm. | 91F205  |        |
|       |   | diox  | O <sub>2</sub>   | 0.6            | PL/LI-56 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.6^b$ ; $\lambda_{exc} = 633$ nm. | 91F205  |        |
| 2.218 | Tetrabenz[b,g,l,q]porphine, 6,13,20-triphenyl-, zinc(II)  | diox  | O <sub>2</sub>   | 0.7            | PL/LI-56 | $S' = HP$ ; rel. to $\phi_{\Delta}(S') = 0.6^b$ ; $\lambda_{exc} = 633$ nm. | 91F205  |        |
| 2.219 | Cadmium(II) chlorotexaphyrin nitrate                      | MeOH  | air              | 0.74           | 0.76     | PL/LI-56,42   | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; meas. $\phi_T(S) = 0.97$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ . | 89A356 |
| 2.220 | Cadmium(II) texaphyrin nitrate                            | MeOH  | air              | 0.69           | 0.78     | PL/LI-56,42   | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; meas. $\phi_T(S) = 0.88$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ . | 89A356 |
| 2.221 | Europium(III) dimethyltexaphyrin dihydroxide              | MeOH  | air              | <0.05          |          | PL/LI-56  | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ .                            | 89A356 |
| 2.222 | Manganese(II) texaphyrin, hydroxide                       | MeOH  | air              | <0.05          |          | PL/LI-56  | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ .                            | 89A356 |
| 2.223 | Samarium(II) dimethyltexaphyrin dihydroxide               | MeOH  | air              | <0.05          |          | PL/LI-56  | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ .                            | 89A356 |
| 2.224 | Zinc(II) chlorotexaphyrin chloride                        | MeOH  | air              | 0.65           | 0.73     | PL/LI-56,42   | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; meas. $\phi_T(S) = 0.88$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ . | 89A356 |
| 2.225 | Zinc(II) texaphyrin chloride                              | MeOH  | air              | 0.61           | 0.74     | PL/LI-56,42   | $S' = T(p-HOP)P$ ; rel. to $\phi_{\Delta}(S') = 0.56$ ; meas. $\phi_T(S) = 0.82$ ; $\lambda_{exc} = 355$ nm. $P_T^{O_2} = 1$ , used $P_S^{O_2} = 0$ . | 89A356 |
| 2.226 | Zinc methyl pyoverdin                                     | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup> | 0.17           |          | PL/LI-56  | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 91R193 |
| 2.227 | Mesoverdin methyl ester                                   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup> | 0.10           |          | PL/LI-56  | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 91R193 |
| 2.228 | Deuteroverdin methyl ester                                | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup> | 0.18           |          | PL/LI-56  | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 91R193 |
| 2.229 | Coproverdin II trimethyl ester                            | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup> | 0.14           |          | PL/LI-56  | $S' = Ac$ ; rel. to $\phi_{\Delta}(S') = 0.84$ ; $\lambda_{exc} = 355$ nm.  | 91R193 |

<sup>a</sup> Oxygen concentration not given; assumed to be air saturated.<sup>b</sup> Value of  $\phi_{\Delta}(S')$  used in this work to calculate  $\phi_{\Delta}(S)$  from authors' reported  $\phi_{\Delta}(S)/\phi_{\Delta}(S')$ .<sup>T</sup> Value corrected for 100% quenching of T<sub>1</sub>.\* Values recalculated using  $\phi_{\Delta}(S')$  or  $f_{\Delta}^T(S')$  from Table 4 or from the quoted reference.

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.

| No.  | Solvent   | [O <sub>2</sub> ] | φ <sub>Δ</sub> | Method   | Comment   | Ref.   |
|------|---|-------------------|----------------|----------|---|--------|
| 3.1  | <b>Anthra[9,1,2-cde]benzo[rsf]pentaphene-5,10-dione (Dibenzanthrone)</b>  |                   |                |          |   |        |
|      | CDCl <sub>3</sub>   | air               | 0.03           | MP/LI-56 | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.2  | <b>Anthra[9,1,2-cde]benzo[rsf]pentaphene-5,10-dione, dibromo-16,17-dimethoxy-</b>   |                   |                |          |   |        |
|      | CDCl <sub>3</sub>   | air               | <0.02          | MP/LI-56 | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.3  | <b>Anthra[9,1,2-cde]benzo[rsf]pentaphene-5,10-dione, 16,17-dinitro-</b>   |                   |                |          |   |        |
|      | CDCl <sub>3</sub>   | air               | <0.02          | MP/LI-56 | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.4  | <b>Anthra[9,1,2-cde]benzo[rsf]pentaphene-10,18-dione, 6,15-dichloro-</b>  |                   |                |          |   |        |
|      | CCl <sub>4</sub>  | air               | 0.2            | MP/LI-56 | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
|      | CDCl <sub>3</sub>   | air               | 0.085          | MP/LI-56 | S' = TPP; rel. to φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.5  | <b>Anthra[2,1-d:6,5-d']bisthiazole-6,12-dione, 1,8-diphenyl-</b>  |                   |                |          |   |        |
|      | EtOH/C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>    | 0.51           | CP/Oc-27 | A = Furan; λ <sub>exc</sub> = 365 nm.   | 73F677 |
| 3.6  | <b>2-Anthracesulfonic acid, 1-amino-9,10-dihydro-9,10-dioxo-4-[3-[(2-(sulfoxy)ethyl)sulfonyl]phenyl]amino]-, disodium salt</b>          |                   |                |          |   |        |
|      | 2-PrOH/ H <sub>2</sub> O (10:1)   | air               | 0.017          | CP/Ac-45 | S' = RB; A = DMA; rel. to φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.7  | <b>Benzenesulfonic acid, 2-[(4-amino-3-bromo-9,10-dihydro-9,10-dioxo-1-anthracenyl)amino]-5-methyl-, monosodium salt</b>                |                   |                |          |   |        |
|      | 2-PrOH/ H <sub>2</sub> O (10:1)   | air               | 0.015          | CP/Ac-45 | S' = RB; A = DMA; rel. to φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.8  | <b>Benzenesulfonic acid, 4-[(4-amino-9,10-dihydro-9,10-dioxo-1-anthracenyl)amino]phenyl]amino]-6-(2-chloro-1,3,5-triazin-4-yl)amino</b> |                   |                |          |   |        |
|      | 2-PrOH/ H <sub>2</sub> O (10:1)   | air               | 0.014          | CP/Ac-45 | S' = RB; A = DMA; rel. to φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.9  | <b>Benzenesulfonic acid, 4-[(2-methoxy-5-(2-sulfatoethyl)sulfonylphenyl]azo-3-[2-hydroxy-5-methyl-imidaz-1-yl]-, disodium salt</b>      |                   |                |          |   |        |
|      | 2-PrOH/ H <sub>2</sub> O (10:1)   | air               | >0.1           | CP/Ac-45 | S' = RB; A = DMA; rel. to φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.10 | <b>Benzimidazo[2,10a]benz[de]isoquinolin-7-one, 4-benzoyl-</b>  |                   |                |          |   |        |
|      | CHCl <sub>3</sub>   | air <sup>a</sup>  | 0.55           | PL/LI-56 | S' = MPDEE; rel. to φ <sub>Δ</sub> (S') = 0.77. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F631 |
|      | EtOH  | air <sup>a</sup>  | 0.56           | CP/Oc-43 | S' = MPDEE; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to φ <sub>Δ</sub> (S') = 0.77. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0. | 82F631 |
| 3.11 | <b>Benzo[d]naphtho[1,2-b]pyran-6-one, 4-(6-deoxy-α-galactofuranosyl)-1-hydroxy-10,12-dimethoxy-8-methyl- (Gilvocarcin V)</b>            |                   |                |          |   |        |
|      | DMSO  | air               | 0.15           | CP/Pa-43 | S' = RB; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethyl-piperidine N-oxyl; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 405 nm.   | 89D112 |
| 3.12 | <b>Benzo[a]phenothiazinium, 5-amino-9-diethylamino-</b>   |                   |                |          |   |        |
|      | MeOH  | air <sup>a</sup>  | 0.024          | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid.  | 87R190 |
| 3.13 | <b>Benzo[a]phenothiazinium, 5-amino-9-diethylamino-6-iodo-</b>  |                   |                |          |   |        |
|      | MeOH  | air <sup>a</sup>  | 0.28           | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76. Acidic soln.; data from Cincotta (unpubl.).  | 90E288 |
|      | MeOH  | air <sup>a</sup>  | 0.17           | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid.  | 87R190 |
| 3.14 | <b>Benzo[a]phenothiazinium, 5-benzylamino-9-diethylamino-</b>   |                   |                |          |   |        |
|      | MeOH  | air <sup>a</sup>  | 0.021          | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid.  | 87R190 |
| 3.15 | <b>Benzo[a]phenoxyazinium, 5-amino-6-bromo-9-diethylamino-</b>  |                   |                |          |   |        |
|      | MeOH  | air <sup>a</sup>  | 0.007          | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid.  | 87R190 |
| 3.16 | <b>Benzo[a]phenoxyazinium, 5-amino-6,8-dibromo-9-ethylamino-</b>  |                   |                |          |   |        |
|      | MeOH  | air <sup>a</sup>  | 0.082          | CP/Ac-45 | S' = RB; A = DPBF; rel. to φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid.  | 87R190 |

## QUANTUM YIELDS FOR FORMATION OF SINGLET OXYGEN

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Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent  | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment  | Ref.   |
|------|--|-------------------|----------------|----------|--|--------|
| 3.17 | Benzo[ <i>a</i> ]phenoxazinium, 5-amino-9-diethylamino-  |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.005          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.18 | Benzo[ <i>a</i> ]phenoxazinium, 5-amino-9-diethylamino-2,6-diiodo-   |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.034          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.19 | Benzo[ <i>a</i> ]phenoxazinium, 5-amino-9-ethylamino-6,8-diiodo-   |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.50           | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.20 | Benzo[ <i>a</i> ]phenoxazinium, 5-amino-9-diethylamino-2-iodo-   |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.008          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.21 | Benzo[ <i>a</i> ]phenoxazinium, 5-amino-9-diethylamino-6-iodo-   |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.06           | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76. Acidic soln.; data from Cincotta (unpubl.).               | 90E288 |
|      | MeOH   | air <sup>a</sup>  | 0.036          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.22 | Benzo[ <i>a</i> ]phenoxazinium, 5-benzylamino-9-diethylamino-  |                   |                |          |  |        |
|      | MeOH   | air <sup>a</sup>  | 0.005          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 630 nm. Soln. cont. 0.04% acetic acid. | 87R190 |
| 3.23 | 1,2-Benzothiazine-3-carboxamide, 4-hydroxy-2-methyl- <i>N</i> -(2-pyridyl)- 1,1-dioxide (Piroxicam)  |                   |                |          |  |        |
|      | C <sub>6</sub> H <sub>6</sub>  | air               | <0.02          | PL/LI-56 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.29; λ <sub>exc</sub> = 308 nm. No emission detected.                    | 91F273 |
|      | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>  | ≤0.01          | PL/LI-56 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 355 nm.  | 87R130 |
|      | D <sub>2</sub> O pH = -7   | air <sup>a</sup>  | ≤0.002         | PL/LI-56 | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 265, 355 nm.    | 87R130 |
| 3.24 | 1,2-Benzothiazin-4-one, 2,3-dihydro-2-methyl-, 1,1-dioxide   |                   |                |          |  |        |
|      | C <sub>6</sub> H <sub>6</sub>  | air <sup>a</sup>  | 0.40*          | PL/LI-56 | S' = Ac; rel. to Φ <sub>Δ</sub> (S') = 0.73; λ <sub>exc</sub> = 355 nm.  | 87R130 |
|      |  |                   | 0.35           |          |  |        |
|      | D <sub>2</sub> O pH = -7   | air <sup>a</sup>  | 0.20           | PL/LI-56 | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 265 nm.         | 87R130 |
|      | D <sub>2</sub> O pH = -7   | air <sup>a</sup>  | 0.18           | PL/LI-56 | S' = H <sub>2</sub> TMpyP <sup>4+</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.74; λ <sub>exc</sub> = 355 nm.         | 87R130 |
| 3.25 | Benzothiazolium, 5-chloro-2-[2-[3-[(5-chloro-3-ethyl-2-benzothiazolidene)ethylidene]-2-(diphenylamino)-1-cyclopenten-1-yl]ethenyl]-3-ethyl-perchlorate |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.014          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |
| 3.26 | Benzothiazolium, 6-chloro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate                             |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.017          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |
| 3.27 | Benzothiazolium, 3,6-dimethyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate                                  |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.012          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |
| 3.28 | Benzothiazolium, 6-fluoro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate                             |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.012          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |
| 3.29 | Benzothiazolium, 6-methoxy-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate                            |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.006          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |
| 3.30 | Benzothiazolium, 3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1,3,5-heptatrienyl]-, iodide   |                   |                |          |  |        |
|      | Propylene carbonate  | O <sub>2</sub>    | 0.017          | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.                  | 87E690 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent                                       | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment   | Ref.   |
|--|---|-------------------|----------------|----------|---|--------|
| <b>3.31 5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)-α-methyl- (Benoxyprofen)</b>  |   |                   |                |          |   |        |
|  | H <sub>2</sub> O pH = 8.0                     | air               | 0.18           | CP/Oc-14 | A = His'. Assumed Φ <sub>ox</sub> = Φ <sub>Δ</sub> in the presence of 0.1 mol L <sup>-1</sup> His, but measured Φ <sub>T</sub> = 0.19 was reduced by 2.6 in the presence of His. Thus 2.6 × Φ <sub>ox</sub> = Φ <sub>Δ</sub> in the absence of His. | 85E163 |
| <b>3.32 3-Benzoxazolepropanesulfonic acid, 2-[4-(1,3-dibutyltetrahydro-4,6-dioxo-2-thioxo-5-pyrimidinylidene)-2-butenyldene]-, sodium salt (Merocyanine 540)</b> |   |                   |                |          |   |        |
|  | H <sub>2</sub> O (ves)                        | O <sub>2</sub>    | 0.015-0.05     | CP/Ac-43 | A = DMA; λ <sub>exc</sub> = 376 nm. rel. to Φ <sub>Δ</sub> (MC540) in EtOH = 0.007; DMPC liposomes  | 91R140 |
|  | H <sub>2</sub> O (ves)                        | O <sub>2</sub>    | 0.035-0.05     | CP/Ac-43 | S' = RB; A = ADPA; rel. to Φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 376 nm. DMPC liposomes; rel. to S' in H <sub>2</sub> O; at 38°C Φ <sub>Δ</sub> increases by factor of 1.3   | 91R140 |
|  | D <sub>2</sub> O/MeOD (1:1)                   | air <sup>a</sup>  | 0.02           | PL/LI-56 | S' = Ery; rel. to Φ <sub>Δ</sub> (S') = 0.60.   | 91A208 |
|  | H <sub>2</sub> O/EtOH (94:6)                  | O <sub>2</sub>    | 0.003          | CP/Oc-43 | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 568 nm. λ <sub>exc</sub> = 550 for RB.   | 91R063 |
|  | EtOH  | air               | 0.007          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.86.  | 88F151 |
|  | MeOH  | air               | 0.004          | CP/Ac-45 | S' = RB; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.86. Rel. to S' in ethanol.   | 88F151 |
|  | CD <sub>3</sub> OD                            | O <sub>2</sub>    | 0.03           | PL/LI-56 | S' = T(m-HOP)P; rel. to Φ <sub>Δ</sub> (S') = 0.57; λ <sub>exc</sub> = 532 nm. P <sub>T</sub> <sup>O</sup> = 1.   | 91R017 |
| <b>3.33 Biline-8,12-dipropionic acid, 18-ethenyl-3-ethylidene-1,2,3,15,16,19,22,24-octahydro-2,7,13,17-tetramethyl-1,19-dioxo-, dimethyl ester</b>               |   |                   |                |          |   |        |
|  | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air               | 0.0008         | CP/Ac-14 | A = DPBF; λ <sub>exc</sub> = 597 nm.  | 91R184 |
| <b>3.34 (2,2'-Bipyridine)bis(bromo)platinum(II)</b>  |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.05. Obs. P by esr.   | 88A276 |
| <b>3.35 (2,2'-Bipyridine)bis(chloro)platinum(II)</b>   |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.19. Obs. P by esr.   | 88A276 |
| <b>3.36 (2,2'-Bipyridine)bis(cyano)platinum(II)</b>  |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.31. Obs. P by esr.   | 88A276 |
| <b>3.37 (2,2'-Bipyridine)bis(iodo)platinum(II)</b>   |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OI; P = 4-IHydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.02. Obs. P by esr.  | 88A276 |
| <b>3.38 (2,2'-Bipyridine)bis(thiocyanato)platinum(II)</b>  |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.16. Obs. P by esr.   | 88A276 |
| <b>3.39 2,2'-Bipyridine(2,3-naphthalenediolato)palladium(II)</b>   |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dhn); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.04. Obs. P by esr.  | 91F203 |
| <b>3.40 2,2'-Bipyridine(2,3-naphthalenediolato)platinum(II)</b>  |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dhn); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.15. Obs. P by esr   | 91F203 |
| <b>3.41 2,2'-Biquinoline(2,3-naphthalenediolato)palladium(II)</b>  |   |                   |                |          |   |        |
|  | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dhn); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.05. Obs. P by esr   | 91F203 |

## QUANTUM YIELDS FOR FORMATION OF SINGLET OXYGEN

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Table 3, Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent  | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment   | Ref.   |
|------|--|-------------------|----------------|----------|---|--------|
| 3.42 | 2,2'-Biquinoline(2,3-naphthalenediolato)platinum(II)   |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dln); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.07. Obs. P by esr       | 91F203 |
| 3.43 | Bis(azido)(2,2'-biquinoline)palladium(II)  |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.04. Obs. P by esr. | 90F196 |
| 3.44 | Bis(azido)(2,2'-biquinoline)platinum(II)   |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.05. Obs. P by esr. | 90F196 |
| 3.45 | Bis(azido)(2,2'-bipyridine)palladium(II)   |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.18. Obs. P by esr. | 90F196 |
| 3.46 | Bis(azido)(4,7-diphenyl-1,10-phenanthroline)palladium(II) Pd(4,7-Ph <sub>2</sub> phen)(N <sub>3</sub> ) <sub>2</sub> |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.34. Obs. P by esr. | 90F196 |
| 3.47 | Bis(azido)(4,7-diphenyl-1,10-phenanthroline)platinum(II) Pt(4,7-Ph <sub>2</sub> phen)(N <sub>3</sub> ) <sub>2</sub>  |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.76. Obs. P by esr. | 90F196 |
| 3.48 | Bis(azido)(1,10-phenanthroline)palladium(II)   |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.17. Obs. P by esr. | 90F196 |
| 3.49 | Bis(azido)(1,10-phenanthroline)platinum(II)  |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(bpy)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.82. Obs. P by esr. | 90F196 |
| 3.50 | 4- <i>tert</i> -Butylcatechol(1,10-phenanthroline)palladium(II) Pd(phen)(BCAT)                                       |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    | -0.18          | CP/Pa-43 | S' = Pt(phen)(BCAT); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = -0.15 <sup>b</sup> . Obs. P by esr.                           | 89F181 |
| 3.51 | 4- <i>tert</i> -Butylcatechol(1,10-phenanthroline)platinum(II) Pt(phen)(BCAT)  |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    | -0.15          | CP/Pa-43 | S' = HP; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = 0.6 <sup>b</sup> . Obs. P by esr.   | 89F181 |
| 3.52 | 4,4'-Carbocyanine, 1,1'-diethyl- (Kryptocyanine)   |                   |                |          |   |        |
|      | D <sub>2</sub> O (mic) pH = -7   | O <sub>2</sub>    | <0.03          | PL/LI-56 | S' = T(m-HOP)P; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 355, 532 nm. Triton X-100; same results for HSA-bound dye.   | 90R164 |
|      | H <sub>2</sub> O (cells)   | O <sub>2</sub>    | <0.05          | PL/LI-56 | S' = T(m-HOP)P; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 355, 532 nm.   | 90R164 |
|      | MeOD   | O <sub>2</sub>    | <0.02          | PL/LI-56 | S' = T(m-HOP)P; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 355, 532 nm. P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0, P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.       | 90R164 |
| 3.53 | Catechol(1,10-phenanthroline)palladium(II) Pd(phen)(CAT)   |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    | -0.09          | CP/Pa-43 | S' = Pt(phen)(BCAT); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = -0.15 <sup>b</sup> . Obs. P by esr.                           | 89F181 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent  | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment   | Ref.   |
|------|--|-------------------|----------------|----------|---|--------|
| 3.54 | Catechol(1,10-phenanthroline)platinum(II) Pt(phen)(CAT)  |                   |                |          |   |        |
|      | DMF  | O <sub>2</sub>    | ~0.07          | CP/Pa-43 | S' = Pt(phen)(BCAT); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = ~0.15 <sup>b</sup> . Obs. P by esr.                                     | 89F181 |
| 3.55 | Cobrynic acid, bis(cyano)-7-de(carboxymethyl)-7,8-didehydro-, hexamethyl ester   |                   |                |          |   |        |
|      | C <sub>6</sub> D <sub>6</sub>  | O <sub>2</sub>    | 0.13           | CP/Ac-14 | A = DMA; λ <sub>exc</sub> = 710 nm.   | 83F222 |
|      | C <sub>6</sub> H <sub>6</sub>  | O <sub>2</sub>    | 0.13           | CP/Ac-14 | A = DMA; λ <sub>exc</sub> = 710 nm.   | 83F222 |
|      | CDCl <sub>3</sub>  | O <sub>2</sub>    | 0.12           | CP/Ac-14 | A = DMA; λ <sub>exc</sub> = 710 nm.   | 83F222 |
|      | CHCl <sub>3</sub>  | O <sub>2</sub>    | 0.12           | CP/Ac-14 | A = DMA; λ <sub>exc</sub> = 710 nm.   | 83F222 |
|      | MeOD   | O <sub>2</sub>    | 0.18           | CP/Ac-14 | A = DMA; λ <sub>exc</sub> = 710 nm.   | 83F222 |
| 3.56 | Diazene, 1-(4-acetylamino-5-hydroxy-2-methylphenyl)-2-phenyl-  |                   |                |          |   |        |
|      | CHCl <sub>3</sub>  | air <sup>a</sup>  | 0.04           | PL/LI-56 | S' = MPDEE; rel. to Φ <sub>Δ</sub> (S') = 0.77. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F631 |
|      | EtOH   | air <sup>a</sup>  | 0.05           | CP/Oc-43 | S' = MPDEE; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.77. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.     | 82F631 |
| 3.57 | Diazene, 1-(2-bromo-6-cyano-4-nitrophenyl)-2-[2-(acetylamino)-4-[N-(2-cyanoethyl)-N-(2-hydroxyethyl)amino]-5-methoxyphenyl]- |                   |                |          |   |        |
|      | Dibutyl terephthalate  | air <sup>a</sup>  | -0.0007        | CP/Ac-43 | A = TPCP; λ <sub>exc</sub> = 589 nm. Rel. to Φ <sub>Δ</sub> (TPP) = 0.74 and Φ <sub>Δ</sub> (ZnTPP) = 0.79 in pyridine. Short lifetime indicates P <sub>T</sub> <sup>O<sub>2</sub></sup> < 1. | 81F609 |
| 3.58 | Diazene, 1-(2-bromo-4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[N-(2-cyanoethyl)-N-(2-hydroxyethyl)amino]-5-methoxyphenyl]-     |                   |                |          |   |        |
|      | Dibutyl terephthalate  | air <sup>a</sup>  | -0.0007        | CP/Ac-43 | A = TPCP; λ <sub>exc</sub> = 589 nm. Rel. to Φ <sub>Δ</sub> (TPP) = 0.74 and Φ <sub>Δ</sub> (ZnTPP) = 0.79 in pyridine. Short lifetime indicates P <sub>T</sub> <sup>O<sub>2</sub></sup> < 1. | 81F609 |
| 3.59 | Diazene, 1-(2-chloro-4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[N-(2-cyanoethyl)-N-(2-hydroxyethyl)amino]-5-methoxyphenyl]-    |                   |                |          |   |        |
|      | Dibutyl terephthalate  | air <sup>a</sup>  | -0.0007        | CP/Ac-43 | A = TPCP; λ <sub>exc</sub> = 589 nm. Rel. to Φ <sub>Δ</sub> (TPP) = 0.74 and Φ <sub>Δ</sub> (ZnTPP) = 0.79 in pyridine. Short lifetime indicates P <sub>T</sub> <sup>O<sub>2</sub></sup> < 1. | 81F609 |
| 3.60 | Diazene, 1-(4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[N-(2-cyanoethyl)-N-(2-hydroxyethyl)amino]-5-methoxyphenyl]-             |                   |                |          |   |        |
|      | Dibutyl terephthalate  | air <sup>a</sup>  | -0.0007        | CP/Ac-43 | A = TPCP; λ <sub>exc</sub> = 589 nm. Rel. to Φ <sub>Δ</sub> (TPP) = 0.74 and Φ <sub>Δ</sub> (ZnTPP) = 0.79 in pyridine. Short lifetime indicates P <sub>T</sub> <sup>O<sub>2</sub></sup> < 1. | 81F609 |
| 3.61 | Diazene, 1-(4-methylphenyl)-2-[1-(phenylaminocarbonyl)-2-oxopropyl]-   |                   |                |          |   |        |
|      | DMAA   | air               | <0.0022        | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
|      | DMF  | air               | <0.012         | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.   | 86F622 |
|      | DMF  | air               | <0.0021        | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
| 3.62 | Diazene, 1-phenyl-2-[1-(phenylaminocarbonyl)-2-oxopropyl]-   |                   |                |          |   |        |
|      | DMAA   | air               | <0.026         | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
|      | DMF  | air               | <0.024         | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.   | 86F622 |
|      | DMF  | air               | <0.023         | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
|      | 2-PrOH   | air               | ≤0.022         | CP/Ac-43 | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
| 3.63 | Dibenz[f,i,j]isoquinoline-2,7-dione, 3-methyl-6-(phenylamino)-   |                   |                |          |   |        |
|      | CHCl <sub>3</sub>  | air <sup>a</sup>  | 0.008          | PL/LI-56 | S' = MPDEE; rel. to Φ <sub>Δ</sub> (S') = 0.77. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 82F631 |
|      | EtOH   | air <sup>a</sup>  | 0.02           | CP/Oc-43 | S' = MPDEE; A = H <sub>2</sub> NCSNH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.77. Assumed P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1, P <sub>S</sub> <sup>O<sub>2</sub></sup> = 0.     | 82F631 |
| 3.64 | Dibenzo[def,mno]chrysene-6,12-dione, 4,10-dibromo-   |                   |                |          |   |        |
|      | CCl <sub>4</sub>   | air               | 0.75*          | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
|      |  |                   | 0.85           |          |   |        |
| 3.65 | 2,3:7,8-Dibenzopyrene-1,6-dione  |                   |                |          |   |        |
|      | C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub>  | air <sup>a</sup>  | 0.77           | PL/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90F577 |
|      | CH <sub>3</sub> CN   | air <sup>a</sup>  | 0.70           | PL/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90F577 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent   | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment   | Ref.             |
|------|---|-------------------|----------------|----------|---|------------------|
| 3.65 | 2,3:7,8-Dibenzopyrene-1,6-dione                                       | —Continued        |                |          |   |                  |
|      | CCl <sub>4</sub>  | air               | 0.7*           | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863           |
|      |   |                   | 0.8            |          |   |                  |
|      | EtOH  | air <sup>a</sup>  | 0.63           | PL/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 90F577           |
|      | EtOH/C <sub>6</sub> H <sub>6</sub>                                    | O <sub>2</sub>    | 0.62           | CP/Oc-27 | A = Furan; λ <sub>exc</sub> = 365 nm.   | 73F677           |
|      | D <sub>2</sub> O  | air <sup>a</sup>  | -0.09          | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Aggregates present.   | 90F577           |
|      | D <sub>2</sub> O/EtOH (75:25)   | air <sup>a</sup>  | -0.1           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90F577           |
| 3.66 | 2,3:7,8-Dibenzopyrene-1,6-dione, 4,9-dibromo-                         |                   |                |          |   |                  |
|      | CCl <sub>4</sub>  | air               | 0.84*          | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863           |
|      |   |                   | 0.95           |          |   |                  |
| 3.67 | 2,3:7,8-Dibenzopyrene-1,6-dione, 4,9-dichloro-                        |                   |                |          |   |                  |
|      | CDCl <sub>3</sub>   | air               | 0.65           | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863           |
| 3.68 | Dibromo(1,10-phenanthroline)platinum(II)                              |                   |                |          |   |                  |
|      | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(phen)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.07. Obs. P by esr.  | 88A276           |
| 3.69 | Dichloro(1,10-phenanthroline)platinum(II)                             |                   |                |          |   |                  |
|      | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(phen)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.19. Obs. P by esr.  | 88A276           |
| 3.70 | Dicyano(1,10-phenanthroline)platinum(II)                              |                   |                |          |   |                  |
|      | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(phen)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.41. Obs. P by esr.  | 88A276           |
| 3.71 | Dihematoporphyrin ester   |                   |                |          |   |                  |
|      | D <sub>2</sub> O  | O <sub>2</sub>    | 0.4            | PL/LI-56 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> ; λ <sub>exc</sub> = 355 nm.  | 86E061           |
|      | D <sub>2</sub> O (mic)  | O <sub>2</sub>    | 0.6            | PL/LI-56 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.4 <sup>b</sup> ; λ <sub>exc</sub> = 355 nm. Soln. cont. 0.01 mol L <sup>-1</sup> CTAB.   | 86E061           |
|      | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.29           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; meas. φ <sub>T</sub> (S) = 0.90; λ <sub>exc</sub> = 347 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1; CTAB micelles; detd. mol. wt. of DHE of = 4200.                 | 86F541<br>87R188 |
|      | MeOD  | air <sup>a</sup>  | 0.30           | PL/LI-56 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.64; λ <sub>exc</sub> = 347 nm. Reported Φ <sub>Δ</sub> = 0.25, using Φ <sub>Δ</sub> (S') = 0.53; recalcd. using Φ <sub>Δ</sub> (S') from [88Z155]; detd. mol. wt. of DHE of = 4200.                          | 87R188           |
| 3.72 | Dihematoporphyrin ester chlorin                                       |                   |                |          |   |                  |
|      | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.23           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; meas. φ <sub>T</sub> (S) = 1; λ <sub>exc</sub> = 347 nm. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.  | 87R188<br>86F541 |
|      | MeOD  | air <sup>a</sup>  | 0.30           | PL/LI-56 | S' = HP; rel. to Φ <sub>Δ</sub> (S') = 0.64; meas. φ <sub>T</sub> (S) = 0.85; λ <sub>exc</sub> = 347 nm. Reported Φ <sub>Δ</sub> = 0.25, using Φ <sub>Δ</sub> (S') = 0.53; recalcd. using Φ <sub>Δ</sub> (S') from [88Z155]; assumed mol. wt. = 1200. | 87R188<br>86F541 |
| 3.73 | Diiodo(1,10-phenanthroline)platinum(II)                               |                   |                |          |   |                  |
|      | DMF   | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pt(phen)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.04. Obs. P by esr.  | 88A276           |
| 3.74 | 3,4-Dimercaptotoluene(1,10-phenanthroline)palladium(II) Pd(phen)(DMT) |                   |                |          |   |                  |
|      | DMF   | O <sub>2</sub>    | -0.01          | CP/Pa-43 | S' = Pt(phen)(BCAT); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = -0.15 <sup>b</sup> . Obs. P by esr.   | 89F181           |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.  | Solvent   | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment  | Ref.             |
|------|---|-------------------|----------------|----------|--|------------------|
| 3.75 | Dinaphtho[2,3-a:2',3'-i]carbazole-4,9-diamine, N,N'-dibenzoyl-10,15,16,17-tetrahydro-5,10,15,17-tetraoxo- |                   |                |          |  |                  |
|      | CDCl <sub>3</sub>   | air               | 0.2            | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.   | 85E863           |
| 3.76 | 4,7-Diphenyl-1,10-phenanthroline(2,3-naphthalenediolato)platinum(II) Pt(4,7-Ph <sub>2</sub> phen)(dnt)    | DMF               | O <sub>2</sub> | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dnt); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.63. Obs. P by esr                    | 91F203           |
| 3.77 | Fulvic acids  |                   |                |          |  |                  |
|      | H <sub>2</sub> O pH = 4.1-8.6   | air               | 0.014-0.093    | CP/Ac-14 | A = 2,5-DMF; λ <sub>exc</sub> = 366 nm. In various natural waters.   | 777245           |
|      | H <sub>2</sub> O pH = 3.5-10.5  | O <sub>2</sub>    | 0.010-0.030    | CP/Oc-14 | A = FFA.   | 87F139           |
| 3.78 | Hematoporphyrin derivative (Photofrin I)  |                   |                |          |  |                  |
|      | D <sub>2</sub> O  | air <sup>a</sup>  | 0.25           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
|      | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.77           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. contg. 2% Triton X-100.  | 89E729           |
|      | D <sub>2</sub> O (mic)  | O <sub>2</sub>    | 0.35           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 355 nm. Soln. cont. 10 <sup>-2</sup> mol L <sup>-1</sup> CTAB.                                   | 88R204           |
|      | EtOH  | air <sup>a</sup>  | 0.77           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
|      | EtOH  | air <sup>a</sup>  | 0.75           | CP/Ac-14 | A = DPBF; λ <sub>exc</sub> = 620 nm. Assumed f <sub>r</sub> <sup>A</sup> = 2.  | 76R193           |
|      | H <sub>2</sub> O  | air <sup>a</sup>  | 0.12           | CP/Oc-14 | A = FFA; λ <sub>exc</sub> = 405 nm. Used f <sub>r</sub> <sup>A</sup> = 1.23; Φ <sub>Δ</sub> = 0.061, 0.037, 0.067 and 0.05 in soln. contg. 0.9% NaCl excited at 405, 436, 546, and 650 nm, resp. | 85F332           |
|      | H <sub>2</sub> O pH = 7.4   | O <sub>2</sub>    | 0.06           | CP/Ac-43 | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 546 nm. RNO as monitor of P.   | 85R008           |
|      | H <sub>2</sub> O (mic) pH = 7.4   | O <sub>2</sub>    | 0.87           | CP/Ac-43 | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 546 nm. RNO as monitor of P; soln. cont. 0.23 mg/mL egg phosphatidylcholine.                 | 85R008           |
|      | MeOH  | air <sup>a</sup>  | 0.83           | CP/Oc-14 | A = FFA; λ <sub>exc</sub> = 405 nm. Used f <sub>r</sub> <sup>A</sup> = 1.52.   | 85F332           |
| 3.79 | Hematoporphyrin dimers  |                   |                |          |  |                  |
|      | D <sub>2</sub> O  | air <sup>a</sup>  | 0.11           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
|      | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.52           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. contg. 2% Triton X-100.  | 89E729           |
|      | EtOH  | air <sup>a</sup>  | 0.60           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
|      | H <sub>2</sub> O pH = 7.0   | O <sub>2</sub>    | 0.29           | CP/Pa-43 | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.   | 89F580           |
| 3.80 | Hematoporphyrin monomer:dimer:oligomer 2:3:9  |                   |                |          |  |                  |
|      | H <sub>2</sub> O pH = 7.0   | O <sub>2</sub>    | 0.14           | CP/Pa-43 | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.   | 89F580           |
| 3.81 | Hematoporphyrin monomer:dimer:oligomer 4:2:1  |                   |                |          |  |                  |
|      | H <sub>2</sub> O pH = 7.0   | O <sub>2</sub>    | 0.40           | CP/Pa-43 | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.   | 89F580           |
| 3.82 | Hematoporphyrin monomer:dimer:oligomer 5:3:4  |                   |                |          |  |                  |
|      | H <sub>2</sub> O pH = 7.0   | O <sub>2</sub>    | 0.28           | CP/Pa-43 | S' = RB; A = His; rel. to Φ <sub>Δ</sub> (S') = 0.75. RNO as monitor of P.   | 89F580           |
| 3.83 | Hematoporphyrin oligomers   |                   |                |          |  |                  |
|      | D <sub>2</sub> O  | air <sup>a</sup>  | 0.06           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
|      | D <sub>2</sub> O (mic)  | air <sup>a</sup>  | 0.49           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm. Soln. contg. 2% Triton X-100.  | 89E729           |
|      | EtOH  | air <sup>a</sup>  | 0.31           | PL/LI-56 | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.  | 89E729           |
| 3.84 | Humic acids   |                   |                |          |  |                  |
|      | H <sub>2</sub> O pH = 7.2-8.0, 13.0   | O <sub>2</sub>    | 0.005-0.026    | CP/Ac-14 | A = FFA; λ <sub>exc</sub> = 366 nm.  | 84F269<br>87F139 |

Table 3, Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]               | Φ <sub>Δ</sub>   | Method          | Comment   | Ref.   |
|-------|---|---------------------------------|------------------|-----------------|---|--------|
| 3.85  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, cobalt(II) salt (Cobalt(II) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.006.  | 88F568 |
| 3.86  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, cobalt(III) salt (Co(III) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.006.  | 88F568 |
| 3.87  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, chromium(III) salt (Cr(III) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 14.  | 88F568 |
| 3.88  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, copper(II) salt (Cu(II) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.04.  | 88F568 |
| 3.89  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, iron(III) salt (Fe(III) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.4.   | 88F568 |
| 3.90  | Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, nickel(II) salt (Ni(II) Dye II)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye II; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.006.  | 88F568 |
| 3.91  | Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, cobalt(II) salt (Cobalt(II) Dye III)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye III; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.0012.  | 88F568 |
| 3.92  | Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, cobalt(III) salt (Co(III) Dye III)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye III; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.0012.  | 88F568 |
| 3.93  | Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, copper(II) salt (Cu(II) Dye III)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye III; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.0029.   | 88F568 |
| 3.94  | Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, nickel(II) salt (Ni(II) Dye III)   | DMF                             | air <sup>a</sup> | CP/Ac-43        | S' = Zn(II) Dye III; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.0012.  | 88F568 |
| 3.95  | Indolium, 2-[7-(4-bromo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate  | Propylene carbonate             | O <sub>2</sub>   | 0.017 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.96  | Indolium, 2-[7-(4-chloro-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate   | Propylene carbonate             | O <sub>2</sub>   | 0.012 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.97  | Indolium, 2-[7-(4-iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, iodide  | Propylene carbonate             | O <sub>2</sub>   | 0.024 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.98  | Indolium, 2-[7-(4-iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate   | Propylene carbonate             | O <sub>2</sub>   | 0.02 CL/Ac-47   | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.99  | Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-(2,2-dimethoxyethyl)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate                            | Propylene carbonate             | O <sub>2</sub>   | 0.011 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.100 | Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-(1-piperidinio)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, bis(tetrafluoroborate)                            | Propylene carbonate             | O <sub>2</sub>   | 0.022 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.101 | Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-[3-(1,3,3-trimethyl-2-indolylidene)-2-propenyl]-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate | Propylene carbonate             | O <sub>2</sub>   | 0.008 CL/Ac-47  | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.   | 87E690 |
| 3.102 | Indol-3-one, 5-bromo-2-(9-chloro-3-oxonaphtho[1,2- <i>b</i> ]thien-2-ylidene)-4-methyl-1,2-dihydro-   | CDCl <sub>3</sub>               | air              | 0.025 MP/LI-56  | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.103 | Malachite Green cation  | MeOH                            | O <sub>2</sub>   | <0.002 CP/Ac-43 | S' = RB; A = Bu <sub>2</sub> S; rel. to Φ <sub>Δ</sub> (S') = 0.80 <sup>b</sup> ; λ <sub>exc</sub> = 546 nm.<br>Measured P <sub>T</sub> <sup>Q<sub>2</sub></sup> = 1. | 80F304 |
| 3.104 | Mesoporphyrin bound to poly(styrene-co-divinylbenzene)  | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub>   | 0.34 CP/Ac-43   | S' = MPDME; A = BRH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.57.  | 89F267 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent   | [O <sub>2</sub> ]               | Φ <sub>Δ</sub>   | Method        | Comment   | Ref.   |
|-------|---|---------------------------------|------------------|---------------|---|--------|
| 3.105 | Mesoporphyrin di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl] ester bound to poly(styrene-co-divinylbenzene)   | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub>   | 0.02-<br>0.03 | CP/Ac-43<br>S' = MPDME; A = BRH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.57. (0.29 or 0.10) × 10 <sup>-3</sup> mol MP/g resin                                   | 89F267 |
| 3.106 | Mesoporphyrin di[4-(diphenylmethylaminocarbonylphenylmethyl] ester bound to poly(styrene-co-divinylbenzene)   | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub>   | 0.07          | CP/Ac-43<br>S' = MPDME; A = BRH <sub>2</sub> ; rel. to Φ <sub>Δ</sub> (S') = 0.57.  | 89F267 |
| 3.107 | Methanaminium, N-[4-[[4-(dimethylamino)phenyl][4-(phenylamino)-1-naphthalenyl]methylen]-2,5-cyclohexadien-1-ylidene]-N-methyl-chloride                        | MeOH                            | O <sub>2</sub>   | 0.006         | CP/Ac-43<br>S' = RB; A = Bu <sub>2</sub> S; rel. to Φ <sub>Δ</sub> (S') = 0.80 <sup>b</sup> ; λ <sub>exc</sub> = 546 nm.<br>Measured P <sub>T</sub> <sup>0</sup> = 1. | 80F304 |
| 3.108 | 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-(Tetracycline)                      | D <sub>2</sub> O pD = 7         | air              | 0.026         | PL/LI-56<br>S' = RF; rel. to Φ <sub>Δ</sub> (S') = 0.30; λ <sub>exc</sub> = 337 nm.   | 87F290 |
| 3.109 | 5,12-Naphthacenedione, 8-acetyl-10[(3-amino-2,3,6-trideoxy-hexopyranosyloxy)-tetrahydro-6,8,11-trihydroxy-1-methoxy-(Daunomycin)                              | D <sub>2</sub> O pH = 7.4       | O <sub>2</sub>   | 0.02          | PL/LI-56,42<br>S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67. f <sub>Δ</sub> <sup>T</sup> = ~0.1-1 depending on φ <sub>T</sub> (S).     | 89B024 |
| 3.110 | 5,12-Naphthacenedione, 8-acetyl-7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-1-methoxy- (S-cis) (Daunomycinone)   | C <sub>6</sub> H <sub>6</sub>   | O <sub>2</sub>   | 0.03          | PL/LI-56,42<br>S' = PPDME; rel. to Φ <sub>Δ</sub> (S') = 0.55. f <sub>Δ</sub> <sup>T</sup> = ~0.1 using meas. φ <sub>T</sub> (S) = 0.038.                             | 89B024 |
| 3.111 | 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyloxy)-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy- (Adriamycin) | D <sub>2</sub> O pH = 7.4       | O <sub>2</sub>   | 0.02          | PL/LI-56,42<br>S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67. f <sub>Δ</sub> <sup>T</sup> = ~0.1-1 depending on φ <sub>T</sub> (S).     | 89B024 |
| 3.112 | 12-Naphthaceneone, 8-acetyl-10[(3-amino-2,3,6-trideoxyhexopyranosyloxy)-tetrahydro-6,7,11-trihydroxy-5-imino-1-methoxy-(5-iminodaunomycin)                    | D <sub>2</sub> O pH = 7.4       | O <sub>2</sub>   | 0.02          | PL/LI-56,42<br>S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67. f <sub>Δ</sub> <sup>T</sup> = ~0.1-1 depending on φ <sub>T</sub> (S).     | 89B024 |
| 3.113 | 2-Naphthaleneacetic acid, 6-methoxy-α-methyl- (Naproxen)  | H <sub>2</sub> O pH = 2, 7      | air              | ~0.2          | CP/Oc-43<br>S' = BXP; A = 2,5-DMF; rel. to Φ <sub>Δ</sub> (S') = 0.18.  | 88R012 |
| 3.114 | 2-Naphthalenecarboxamide, 4-[[4-(aminocarbonyl)phenyl]azo]-3-hydroxy-N-(2-methoxyphenyl)-   | DMF                             | air              | <0.0014       | CP/Ac-43<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.   | 86F622 |
|       |   | DMF                             | air              | <0.0036       | CP/Ac-43<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
| 3.115 | 2-Naphthalenecarboxamide, 3-hydroxy-4-[(4-methylphenyl)azo]-N-phenyl-   | DMF                             | air              | <0.0012       | CP/Ac-43<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.   | 86F622 |
|       |   | DMF                             | air              | <0.011        | CP/Ac-43<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.   | 86F622 |
| 3.116 | 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-(phenylamino)-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[(2-sulfophenyl)azo]-, trisodium salt                      | 2-PrOH/ H <sub>2</sub> O (10:1) | air              | 0.0054        | CP/Ac-45<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.117 | 1-Naphthalenesulfonic acid, 3-[[4-chloro-6-(4-methyl-2-sulfophenyl)amino]-1,3,5-triazin-2-yl]amino-3-(5-sulfophenyl)azo]-, trisodium salt                     | 2-PrOH/ H <sub>2</sub> O (10:1) | air              | 0.0058        | CP/Ac-45<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.118 | 1-Naphthalenesulfonic acid, 5-hydroxy-6-[[2-methoxy-5-[[2-(sulfoxyethyl)sulfonyl]phenyl]azo]-, disodium salt  | 2-PrOH/ H <sub>2</sub> O (10:1) | air              | 0.0048        | CP/Ac-45<br>S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662 |
| 3.119 | 6-Naphthalenesulfonate ion, 1,1'-methylenebis-  | D <sub>2</sub> O                | air <sup>a</sup> | ~0.4          | PL/LI-56<br>S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.70; λ <sub>exc</sub> = 337 nm.   | 90F577 |
| 3.120 | 1-Naphthol, 5-[[3-(aminosulfonyl)phenyl]sulfonyl]amino]-4-[2-(methylsulfonyl)-4-nitrophenylazo]-, conjugate base  | DMF                             | air              | 0.0037        | CP/Ac-14,A18<br>A = DPBF.   | 79F412 |
|       |   | H <sub>2</sub> O                | air              | 0.00013       | CP/Ac-14,A18<br>A = 2,5-DMF.  | 79F412 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent  | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method       | Comment  | Ref.   |
|-------|--|-------------------|----------------|--------------|--|--------|
| 3.120 | 1-Naphthol, 5-[3-(aminosulfonyl)phenyl]sulfonylamino]-4-[2-(methylsulfonyl)-4-nitrophenylazo]-, conjugate base—Continued |                   |                |              |  |        |
|       | MeOH   | air               | 0.0016         | CP/Ac-14,A18 | A = DPBF.  | 79F412 |
| 3.121 | 1-Naphthol, 5-methoxy-4-[2-(methylsulfonyl)-4-nitrophenyl]azo-, conjugate base   |                   |                |              |  |        |
|       | DMF  | air               | 0.00027        | CP/Ac-14,A18 | A = DPBF.  | 79F412 |
| 3.122 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, aluminum(III) salt (Al(III) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 370.   | 88F568 |
| 3.123 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, chromium(III) salt (Cr(III) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 16.  | 88F568 |
| 3.124 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, cobalt(II) salt (Co(II) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.07.   | 88F568 |
| 3.125 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, cobalt(III) salt (Co(III) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.07.   | 88F568 |
| 3.126 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, copper(II) salt (Cu(II) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.07.   | 88F568 |
| 3.127 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, iron(III) salt (Fe(III) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 2.6.   | 88F568 |
| 3.128 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, nickel(II) salt (Ni(II) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = <0.07.   | 88F568 |
| 3.129 | 2-Naphthol, 1-(2-hydroxyphenylazo)-, zinc(II) salt (Zn(II) Dye I)  |                   |                |              |  |        |
|       | DMF  | air <sup>a</sup>  |                | CP/Ac-43     | S' = Cd(II) Dye I; A = DPBF; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.84.  | 88F568 |
| 3.130 | 2-Naphthol, 1-(4-methyl-2-nitrophenylazo)-   |                   |                |              |  |        |
|       | DMAA   | air               | <0.0031        | CP/Ac-43     | S' ~ RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
|       | DMF  | air               | <0.0056        | CP/Ac-43     | S' ~ RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.  | 86F622 |
|       | DMF  | air               | <0.013         | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
|       | 2-PrOH   | air               | <0.0019        | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
| 3.131 | 2-Naphthol, 1-(4-nitrophenylazo)-  |                   |                |              |  |        |
|       | DMAA   | air               | <0.0046        | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
|       | DMF  | air               | <0.0077        | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
|       | DMF  | air               | <0.0051        | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 564 nm.  | 86F622 |
|       | 2-PrOH   | air               | ≤0.0012        | CP/Ac-43     | S' = RB; A = DMA; rel. to Φ <sub>Δ</sub> (S') = 1; λ <sub>exc</sub> = 435 nm.  | 86F622 |
| 3.132 | Naphtho[1,8- <i>bc</i> ]thiopyran-3-one, 2-(1-oxonaphtho[2,1- <i>b</i> ]thiophen-2-ylidene)-, ( <i>E</i> )               |                   |                |              |  |        |
|       | CDCl <sub>3</sub>  | air               | 0.6            | MP/LI-56     | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.   | 85E863 |
| 3.133 | 1,8-Naphthyridine-3-carboxylic acid, 1,4-dihydro-1-ethyl-7-methyl-4-oxo- (Nalidixic acid)                                |                   |                |              |  |        |
|       | D <sub>2</sub> O pH = 4.4  | air <sup>a</sup>  | 0.24           | PL/LI-56     | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 347 nm. pK <sub>a</sub> = 6.1; Φ <sub>Δ</sub> decreases to 0.09 on addn. of eumelanin. | 88R070 |
| 3.134 | 1,8-Naphthyridine-3-carboxylic acid, 1,4-dihydro-1-ethyl-7-methyl-4-oxo-, anion  |                   |                |              |  |        |
|       | D <sub>2</sub> O pH = 8.9  | air <sup>a</sup>  | 0.15           | PL/LI-56     | S' = H <sub>2</sub> TPPS <sup>4-</sup> ; rel. to Φ <sub>Δ</sub> (S') = 0.67; λ <sub>exc</sub> = 347 nm.  | 88R070 |
| 3.135 | 2,2'-Oxatricarbocyanine, 3,3'-diethyl-, iodide   |                   |                |              |  |        |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.015          | CL/Ac-47     | S' = MB <sup>+</sup> ; A = DPBF; rel. to Φ <sub>Δ</sub> (S') = 0.35; λ <sub>exc</sub> = 633 nm.  | 87E690 |
| 3.136 | (1,10-Phenanthroline)bis(thiocyanato)platinum(II)  |                   |                |              |  |        |
|       | DMF  | O <sub>2</sub>    |                | CP/Pa-43     | S' = Pt(phen)(N <sub>3</sub> ) <sub>2</sub> ; A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.15. Obs. P by esr.   | 88A276 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent  | [O <sub>2</sub> ] | Φ <sub>Δ</sub> | Method   | Comment   | Ref.   |
|-------|--|-------------------|----------------|----------|---|--------|
| 3.137 | 1,10-Phenanthroline(2,3-naphthalenediolato)palladium(II) Pd(phen)(dnt)                                       |                   |                |          |   |        |
|       | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dhn); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.02. Obs. P by esr | 91F203 |
| 3.138 | 1,10-Phenanthroline(2,3-naphthalenediolato)platinum(II) Pt(phen)(dnt)  |                   |                |          |   |        |
|       | DMF  | O <sub>2</sub>    |                | CP/Pa-43 | S' = Pd(4,7-Ph <sub>2</sub> phen)(dhn); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; meas. Φ <sub>Δ</sub> (S)/Φ <sub>Δ</sub> (S') = 0.13. Obs. P by esr | 91F203 |
| 3.139 | 1,10-Phenanthroline(thiosalicylato)palladium(II) Pd(phen)(TSA)   |                   |                |          |   |        |
|       | DMF  | O <sub>2</sub>    | ~0.03          | CP/Pa-43 | S' = Pt(phen)(BCAT); A = TEMP-4-OH; P = 4-Hydroxy-2,2,6,6-tetramethylpiperidine N-oxyl; rel. to Φ <sub>Δ</sub> (S') = ~0.15 <sup>b</sup> . Obs. P by esr.                     | 89F181 |
| 3.140 | 1,10-Phenanthrolinetris(1-thienyl-4,4,4-trifluoro-1,3-butanedionato)europium(III) Eu(phen)(tta) <sub>3</sub> |                   |                |          |   |        |
|       | CCl <sub>4</sub>   | → ∞               | 0.45           | PL/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7; λ <sub>exc</sub> = 347 nm.   | 91E314 |
| 3.141 | Phenothiazine, 10-(1-azabicyclo[2.2.2]oct-3-ylmethyl)- (Mequitazine)   |                   |                |          |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  | air               | 0.34*<br>0.28  | PL/LI-56 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.29; λ <sub>exc</sub> = 308 nm.   | 91F273 |
| 3.142 | Phenothiazine, 2-chloro-10-dimethylaminopropyl- (Chlorpromazine)   |                   |                |          |   |        |
|       | C <sub>6</sub> H <sub>6</sub>  | air               | 0.33*<br>0.27  | PL/LI-56 | S' = BP; rel. to Φ <sub>Δ</sub> (S') = 0.29; λ <sub>exc</sub> = 308 nm.   | 91F273 |
| 3.143 | 12-(10'-Phenothiazinyl)dodecyl-1-sulfonate ion   |                   |                |          |   |        |
|       | H <sub>2</sub> O (mic)   | O <sub>2</sub>    | 0.095          | CP/Oc-14 | A = S; P = 12-(10'-Phenothiazinyl)dodecyl-1-sulfonate ion 9-sulfoxide.  | 85Z063 |
| 3.144 | Photofrin II   |                   |                |          |   |        |
|       | H <sub>2</sub> O pH = 7.4  | O <sub>2</sub>    | 0.01           | PL/Ac-14 | A = TrpH; λ <sub>exc</sub> = 630 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
|       | H <sub>2</sub> O pH = 7.4  | O <sub>2</sub>    | 0.04           | CP/Pa-43 | S' = RB; A = Im; P = Imidazole endoperoxide; rel. to Φ <sub>Δ</sub> (S') = 0.75; λ <sub>exc</sub> = 540 nm. RNO as monitor for P.   | 88N170 |
|       | H <sub>2</sub> O pH = 7.4  | O <sub>2</sub>    | 0.13           | CP/Oc-14 | A = Im; λ <sub>exc</sub> = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
|       | H <sub>2</sub> O pH = 7.4  | O <sub>2</sub>    | 0.09           | CP/Ac-14 | A = TrpH; λ <sub>exc</sub> = 540 nm. Soln. cont. 1.6% NaCl in phosphate buffer.   | 88N170 |
| 3.145 | Poly(sodium styrenesulfonate-co-2-vinylnaphthalene)  |                   |                |          |   |        |
|       | H <sub>2</sub> O   | O <sub>2</sub>    | 0.25           | CP/Ac-14 | A = C <sub>6</sub> H <sub>5</sub> CH=CH <sub>2</sub> .  | 91F015 |
| 3.146 | Pyran, 4-(dicyanomethylene)-6-(4-dimethylaminostyryl)-2-methyl-  |                   |                |          |   |        |
|       | CCl <sub>4</sub>   | air <sup>a</sup>  | 0.0015         | PL/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 90F568 |
| 3.147 | 8,16-Pyranthrenedione  |                   |                |          |   |        |
|       | CDCl <sub>3</sub>  | air               | 0.8            | MP/LI-56 | S' = TPP; rel. to Φ <sub>Δ</sub> (S') = 0.7.  | 85E863 |
| 3.148 | Pyrazole-3-selone, 4-(aminomethylene)-2,4-dihydro-5-methyl-2-phenyl-, (Z)-                                   |                   |                |          |   |        |
|       | 1-BuOH   | air               | 0.16           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | c-C <sub>6</sub> H <sub>12</sub>   | air               | 0.11           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | CCl <sub>4</sub>   | air               | 0.31           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | CDCl <sub>3</sub>  | air               | 0.16           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | CH <sub>3</sub> CN   | air               | 0.16           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | CHCl <sub>3</sub>  | air               | 0.14           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | EtOH   | air               | 0.096          | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | MeOH   | air               | 0.13           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |
|       | MeOH-d <sub>3</sub>  | air               | 0.13           | CP/Ac-14 | A = S; λ <sub>exc</sub> = 366 nm. P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.  | 85F646 |

## QUANTUM YIELDS FOR FORMATION OF SINGLET OXYGEN

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Table 3, Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent   | [O <sub>2</sub> ] | $\phi_{\Delta}$ | Method         | Comment   | Ref.                       |
|-------|---|-------------------|-----------------|----------------|---|----------------------------|
| 3.148 | Pyrazole-3-selone, 4-(aminomethylene)-2,4-dihydro-5-methyl-2-phenyl-, (Z)—Continued                           |                   |                 |                |   |                            |
|       | 2-ProOH   | air               | 0.12            | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | diox  | air               | 0.14            | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
| 3.149 | Pyrazole-3-thione, 4-(aminomethylene)-2,4-dihydro-5-methyl-2-phenyl-  |                   |                 |                |   |                            |
|       | 1-BuOH  | air               | 0.037           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | c-C <sub>6</sub> H <sub>12</sub>  | air               | 0.033           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | CCl <sub>4</sub>  | air               | 0.15            | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | CDCl <sub>3</sub>   | air               | 0.062           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | CH <sub>3</sub> CN  | air               | 0.055           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | CHCl <sub>3</sub>   | air               | 0.059           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | EtOH  | air               | 0.037           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | MeOH  | air               | 0.033           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | MeOH-d <sub>3</sub>   | air               | 0.038           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | 2-ProOH   | air               | 0.030           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
|       | diox  | air               | 0.071           | CP/Ac-14       | A = S; $\lambda_{exc}$ = 366 nm. $P_T^{O_2}$ = 1.                     | 85F646                     |
| 3.150 | Pyrazol-3-one, 2-(4-bromophenyl)-4-(4-diethylamino-2-methylphenyl)-2,4-dihydro-imino-5-methylcarbamyl-        |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0040          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.151 | Pyrazol-3-one, 2-(4-chlorophenyl)-4-(4-diethylamino-2-methylphenyl)-2,4-dihydro-imino-5-methylcarbamyl-       |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0012          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.152 | Pyrazol-3-one, 4-(4-diethylamino-2-methylphenyl)imino-2,4-dihydro-5-methylcarbamyl-2-(3-methoxyphenyl)-       |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0012          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.153 | Pyrazol-3-one, 4-(4-diethylamino-2-methylphenyl)imino-2,4-dihydro-5-methylcarbamyl-2-(3-methylphenyl)-        |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0008          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.154 | Pyrazol-3-one, 4-[[(4-diethylamino)-2-methylphenyl]imino]-2,4-dihydro-5-methyl-2-phenyl-                      |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0026          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.155 | Pyrazol-3-one, 4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2,4-dihydro-2-(2,4,6-trichlorophenyl)- |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0016          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.156 | Pyrazol-3-one, 4-[[(4-diethylamino)phenyl]imino]-2,4-dihydro-5-methyl-2-phenyl-                               |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0027          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.157 | Pyrazol-3-one, 4-[[(4-dimethylamino)phenyl]imino]-2,4-dihydro-5-methyl-2-phenyl-                              |                   |                 |                |   |                            |
|       | CCl <sub>4</sub>  | O <sub>2</sub>    | 0.0021          | CP/Ac-14       | A = 2M2P.   | 87F542                     |
| 3.158 | Pyrazolo[1',2':2,3][1,2,3]triazolo[4,5-a]phenazin-4-iium, 1,3-dimethyl-                                       |                   |                 |                |   |                            |
|       | c-C <sub>6</sub> H <sub>12</sub>  | air               | 0.21            | CP/Ac-27       | A = DPBF; $\lambda_{exc}$ = 543 nm.                                   | 80F548                     |
|       | CHCl <sub>3</sub>   | air               | 0.037           | CP/Ac-27       | A = DPBF; $\lambda_{exc}$ = 543 nm.                                   | 80F548                     |
|       | CHCl <sub>3</sub> /MeOH (8:2)   | air               | 0.053           | CP/Ac-27       | A = DPBF; $\lambda_{exc}$ = 543 nm.                                   | 80F548                     |
| 3.159 | Pyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]-      |                   |                 |                |   |                            |
|       | MeOH  | air               | 0.004           | CP/Ac-43 or 14 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ . | 90F157<br>90R069<br>88A269 |
| 3.160 | Pyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]-     |                   |                 |                |   |                            |
|       | MeOH  | air               | 0.05            | CP/Ac-43 or 14 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ . | 90F157<br>90R069<br>88A269 |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent  | [O <sub>2</sub> ]               | ϕ <sub>Δ</sub> | Method         | Comment   | Ref.                       |
|-------|--|---------------------------------|----------------|----------------|---|----------------------------|
| 3.161 | Pyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)thiapyran-4-ylidene]-3-propenyl]-MeOH | air                             | 0.0006         | CP/Ac-43 or 14 | S' = MB <sup>+</sup> ; A = DPBF; rel. to ϕ <sub>Δ</sub> (S') = 0.50.  | 90R069                     |
| 3.162 | Pyrylium, 4,4'-(1,3-propenyl)bis[2,6-di(1,1-dimethylethyl)-MeOH  | air                             | 0.0004         | CP/Ac-43 or 14 | S' = MB <sup>+</sup> ; A = DPBF; rel. to ϕ <sub>Δ</sub> (S') = 0.50.  | 90F157<br>90R069<br>88A269 |
| 3.163 | 4-Quinazolinone, 6-amino-2-(fluoromethyl)-3-(2-methylphenyl)- (Afloqualone)                                | C <sub>6</sub> H <sub>6</sub>   | air            | 0.17*<br>0.14  | PL/LI-56<br>S' = BP; rel. to ϕ <sub>Δ</sub> (S') = 0.29; λ <sub>exc</sub> = 308 nm.   | 91F273                     |
| 3.164 | Remazol Brilliant Red 5B   | 2-PrOH/H <sub>2</sub> O (10:1)  | air            | 0.0068         | CP/Ac-45<br>S' = RB; A = DMA; rel. to ϕ <sub>Δ</sub> (S') = 0.5; λ <sub>exc</sub> = 546 nm.   | 79F662                     |
| 3.165 | Rhodamine B cation   | MeOH                            | O <sub>2</sub> | 0.016          | CP/Ac-43<br>S' = RB; A = Bu <sub>2</sub> S; rel. to ϕ <sub>Δ</sub> (S') = 0.80 <sup>b</sup> ; λ <sub>exc</sub> = 546 nm.<br>Measured P <sub>T</sub> <sup>O<sub>2</sub></sup> = 1.   | 80F304                     |
| 3.166 | Rhodamine 6G cation  | C <sub>5</sub> H <sub>5</sub> N | O <sub>2</sub> | 0.12           | CP/Oc-14<br>A = H <sub>2</sub> NCSNH <sub>2</sub> . Assumed f <sub>r</sub> <sup>A</sup> = 2.  | 737347<br>74E522           |
| 3.167 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene)                                      | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.76-<br>0.91  | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol; amount of bound dye varied, 9-284 mg RB/g polymer. | 86P106                     |
| 3.168 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), ammonium salt                       | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.27           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.169 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), sec-butylammonium salt              | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.55           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.170 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), <i>tert</i> -butylammonium salt     | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.64           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.171 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), diethylammonium salt                | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.86           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.172 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), isobutylammonium salt               | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.50           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.173 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), piperidinium salt                   | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.74           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |
| 3.174 | Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), pyridinium salt                     | CH <sub>2</sub> Cl <sub>2</sub> | O <sub>2</sub> | 0.35           | CP/Pa-43<br>S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to ϕ <sub>Δ</sub> (S') = 0.76; λ <sub>exc</sub> = 556 nm. Rel. to S' in methanol.  | 86P106                     |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent                                       | [O <sub>2</sub> ] | $\phi_{\Delta}$ | Method         | Comment  | Ref.             |
|---|---|-------------------|-----------------|----------------|--|------------------|
| <b>3.175 Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), tributylammonium salt</b>   |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.66            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol.   | 86P106           |
| <b>3.176 Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), triethylammonium salt</b>   |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.78            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol.   | 86P106           |
| <b>3.177 Rose Bengal bound to chloromethylated poly(styrene-co-divinylbenzene), trimethylammonium salt</b>  |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.46            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol.   | 86P106           |
| <b>3.178 Rose Bengal bound to poly(styrene-co-vinylbenzyl chloride)</b>   |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.16-0.36       | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol; bound dye varied 51-610 mg RB/1.07 g polymer. | 85F171<br>85F436 |
|   | MeOH (dis)                                    | O <sub>2</sub>    | 0.04-0.41       | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol; bound dye varied 51-610 mg RB/1.07 g polymer. | 85F436           |
| <b>3.179 Rose Bengal bound to poly(styrene-co-vinylbenzyl chloride), pyridinium salt</b>  |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.41            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol.   | 86P106           |
| <b>3.180 Rose Bengal bound to poly(styrene-co-vinylbenzyl chloride), triethylammonium salt</b>  |   |                   |                 |                |  |                  |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | O <sub>2</sub>    | 0.61            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 556$ nm. Rel. to S' in methanol.   | 86P106           |
| <b>3.181 Rose Bengal on Sephadex A resin</b>  |   |                   |                 |                |  |                  |
|   | MeOH  | O <sub>2</sub>    | 0.55            | CP/Ac or Oc-43 | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 86F510           |
| <b>3.182 Rose Bengal polyglycol</b>   |   |                   |                 |                |  |                  |
|   | C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> | air <sup>a</sup>  | 0.30            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 559$ nm. Rel. to S' in methanol.   | 86F463           |
|   | C <sub>6</sub> H <sub>6</sub>                 | air <sup>a</sup>  | 0.40            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 559$ nm. Rel. to S' in methanol.   | 86F463           |
|   | CH <sub>2</sub> Br <sub>2</sub>               | air <sup>a</sup>  | 0.81            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 559$ nm. Rel. to S' in methanol.   | 86F463           |
|   | CH <sub>2</sub> Cl <sub>2</sub>               | air <sup>a</sup>  | 0.76            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 559$ nm. Rel. to S' in methanol.   | 86F463           |
|   | EtOH  | air <sup>a</sup>  | 0.75            | CP/Pa-43       | S' = RB; A = 2,3-Diphenyl-1,4-dioxene; P = 1,2-Ethanediol dibenzoate; rel. to $\phi_{\Delta}(S') = 0.76$ ; $\lambda_{exc} = 559$ nm. Rel. to S' in methanol.   | 86F463           |
| <b>3.183 Safranine cation</b>   |   |                   |                 |                |  |                  |
|   | MeOH  | O <sub>2</sub>    | 0.14            | CP/Ac-43       | S' = RB; A = Bu <sub>2</sub> S; rel. to $\phi_{\Delta}(S') = 0.80^b$ ; $\lambda_{exc} = 546$ nm.<br>Measured $P_1^{O_2} = 1$ .   | 80F304           |
| <b>3.184 Selenopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]-H<sub>2</sub>O/CH<sub>3</sub>OH (9:1)</b> |   |                   |                 |                |  |                  |
|   | air   |                   | ≤0.004          | CP/Ac-43 or 14 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157           |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent  | [O <sub>2</sub> ] | $\phi_{\Delta}$ | Method         | Comment   | Ref.                       |
|-------|--|-------------------|-----------------|----------------|---|----------------------------|
| 3.185 | Selenopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-4-(2-butenyl)]-MeOH  | air               | 0.004           | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157                     |
| 3.186 | Selenopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-4-(2-pentenyl)]-MeOH | air               | 0.001           | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157                     |
| 3.187 | Selenopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]-MeOH     | air               | 0.013           | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ . $\phi_{\Delta}$ same in air- or oxygen-satd. methanol.               | 90F157<br>90R069           |
| 3.188 | Selenopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]-MeOH    | air               | 0.09            | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ . $f_{\Delta}^T = 0.75$ using $\phi_T(S) = 0.12$ but $P_S^{O_2} < 1$ . | 90F157<br>90R069<br>88A269 |
| 3.189 | Sensitox HP resin  |                   |                 |                |   |                            |
|       | MeOH   | O <sub>2</sub>    | 0.25            | CP/Oc-43       | $S' = RB$ ; A = 2,3-Diphenyl-1,4-dioxene; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 86F510                     |
| 3.190 | Sensitox P resin   |                   |                 |                |   |                            |
|       | MeOH   | O <sub>2</sub>    | 0.23            | CP/Ac-43;      | $S' = RB$ ; A = 2,3-Diphenyl-1,4-dioxene; rel. to $\phi_{\Delta}(S') = 0.76$ .  | 86F510                     |
|       |  |                   | 0.22            | CP/Oc-43       |   |                            |
| 3.191 | Telluropyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]ethyl]-MeOH         | air               | 0.006           | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157                     |
| 3.192 | Telluropyrylium, 2,6-bis(1,1-dimethylethyl)-4-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]methyl]-MeOH           | air               | 0.07            | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157                     |
| 3.193 | Telluropyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]-MeOH   | air               | 0.12            | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ . $f_{\Delta}^T = 0.67$ using $\phi_T(S) = 0.18$ but $P_S^{O_2} < 1$ . | 90F157<br>90R069<br>88A269 |
| 3.194 | 2,2'-Thiatricarbocyanine, 3,3'-diethyl-, iodide  |                   |                 |                |   |                            |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.025           | CL/Ac-47       | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm.  | 87E690                     |
| 3.195 | Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]-MeOH       | air               | 0.007           | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157<br>90R069           |
| 3.196 | Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]-MeOH      | air               | 0.07            | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157<br>90R069           |
| 3.197 | Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)thiopyran-4-ylidene]-3-propenyl]-MeOH         | air               | 0.0006          | CP/Ac-43 or 14 | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.50$ .  | 90F157<br>90R069           |
| 3.198 | Tricarbocyanine, 5,5'-dichloro-1,1',3,3,3',3'-hexamethyl-, iodide  |                   |                 |                |   |                            |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.02            | CL/Ac-47       | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm.  | 87E690                     |
| 3.199 | Tricarbocyanine, 5,5'-difluoro-1,1',3,3,3',3'-hexamethyl-, iodide  |                   |                 |                |   |                            |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.014           | CL/Ac-47       | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm.  | 87E690                     |
| 3.200 | Tricarbocyanine, 5,5'-dimethoxy-1,1',3,3,3',3'-hexamethyl-, iodide   |                   |                 |                |   |                            |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.004           | CL/Ac-47       | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm.  | 87E690                     |
| 3.201 | Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, fluoride  |                   |                 |                |   |                            |
|       | Propylene carbonate  | O <sub>2</sub>    | 0.013           | CL/Ac-47       | $S' = MB^+$ ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm.  | 87E690                     |

Table 3. Quantum yields of photosensitized production of singlet oxygen, from drugs, dyes, polymers, etc.—Continued

| No.   | Solvent   | [O <sub>2</sub> ] | $\phi_{\Delta}$ | Method   | Comment   | Ref.   |
|-------|---|-------------------|-----------------|----------|---|--------|
| 3.202 | Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, iodide   |                   |                 |          |   |        |
|       | Propylene carbonate   | O <sub>2</sub>    | 0.015           | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm. | 87E690 |
| 3.203 | Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, perchlorate  |                   |                 |          |   |        |
|       | Propylene carbonate   | O <sub>2</sub>    | 0.015           | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm. | 87E690 |
| 3.204 | Tricarbocyanine, 1,1',3,3,3',3',5,5'-octamethyl-, iodide  |                   |                 |          |   |        |
|       | Propylene carbonate   | O <sub>2</sub>    | 0.015           | CL/Ac-47 | S' = MB <sup>+</sup> ; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.35$ ; $\lambda_{exc} = 633$ nm. | 87E690 |
| 3.205 | Tris(2,2'-bipyridine)ruthenium(II) ion bound to Dowex 50W-X1 resin  |                   |                 |          |   |        |
|       | MeOH  | O <sub>2</sub>    | 0.90            | CL/Pa-14 | A = TME; $\lambda_{exc} = 488$ nm.  | 83N166 |
| 3.206 | Tris(1,10-phenanthroline)ruthenium(II) ion bound to Dowex 50W-X1 resin  |                   |                 |          |   |        |
|       | MeOH  | O <sub>2</sub>    | 0.68            | CL/Pa-14 | A = TME; $\lambda_{exc} = 488$ nm.  | 83N166 |
| 3.207 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetraiodo-, dianion, bound as copoly(styrene-p-vinylbenzyl ester) |                   |                 |          |   |        |
|       | DMF   | air <sup>a</sup>  | 0.34            | CP/Ac-43 | S' = RB; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .   | 88F618 |
| 3.208 | Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5-triiodo-, dianion, bound as copoly(styrene-p-vinylbenzyl ester)     |                   |                 |          |   |        |
|       | DMF   | air <sup>a</sup>  | 0.33            | CP/Ac-43 | S' = RB; A = DPBF; rel. to $\phi_{\Delta}(S') = 0.76$ .   | 88F618 |

<sup>a</sup> Oxygen concentration not given; assumed to be air saturated.<sup>b</sup> Value of  $\phi_{\Delta}(S')$  used in this work to calculate  $\phi_{\Delta}(S)$  from authors' reported  $\phi_{\Delta}(S)/\phi_{\Delta}(S')$ .\* Values recalculated using  $\phi_{\Delta}(S')$  or  $f_{\Delta}^T(S')$  from Table 4 or from the quoted reference.

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## 10. Molecular Formula Index

|                     |  |                      |   |
|---------------------|--|----------------------|---|
| $C_4H_6O_2$         | Biacetyl 1.108   | $C_{10}H_8$          | Azulene 1.70<br>Naphthalene 1.220<br>Naphthalene excimer 1.221  |
| $C_5H_6$            | Cyclopentadiene 1.133  | $C_{10}H_8Br_2N_2Pt$ | (2,2'-Bipyridine)bis(bromo)platinum(II)<br>3.34   |
| $C_5H_{10}O$        | 2-Pentanone 1.230<br>3-Pentanone 1.231   | $C_{10}H_8Cl_2N_2Pt$ | (2,2'-Bipyridine)bis(chloro)platinum(II)<br>3.35  |
| $C_6Cl_4O_2$        | Chloranil 1.102<br>Chloranil/Anisole 1.103<br>Chloranil/Durene 1.104<br>Chloranil/Hexamethylbenzene 1.105<br>Chloranil/1,2,3-Trimethoxybenzene 1.106 | $C_{10}H_8I_2N_2Pt$  | (2,2'-Bipyridine)bis(iodo)platinum(II) 3.37   |
| $C_6H_5ClO_2$       | 4-Chlororesorcinol 1.80<br>Chlorohydroquinone 1.82   | $C_{10}H_{10}O$      | $\alpha$ -Tetralone 1.292   |
| $C_6H_6O_2$         | Resorcinol 1.79<br>Hydroquinone 1.81   | $C_{10}H_{12}N_2O_3$ | Kynurenone 1.78   |
| $C_6H_8$            | 1,3-Cyclohexadiene 1.131   | $C_{10}H_{12}N_2O_4$ | 3-Hydroxykynurenone 1.77  |
| $C_7H_6O$           | Benzaldehyde 1.71  | $C_{10}H_{12}O_2$    | Duroquinone 1.107   |
| $C_7H_8$            | Cycloheptatriene 1.130   | $C_{10}H_{14}O_2$    | Camphorquinone 1.109  |
| $C_7H_{10}S$        | Bicyclo[2.2.1]heptane-2-thione 1.110   | $C_{10}H_{16}$       | 2,6-Dimethyl-2,4,6-octatriene 1.228   |
| $C_7H_{14}O$        | 2,4-Dimethyl-3-pentanone 1.232   | $C_{10}H_{16}S$      | Thiofenchone 1.113<br>Thiocamphor 1.114   |
| $C_8H_6N_2$         | Quinoxaline 1.270  | $C_{11}H_6O_3$       | Allopsoralen 1.11<br>Angelicin 1.12<br>Isopseudopsoralen 1.208<br>Pseudoisopsoralen 1.252<br>Pseudopsoralen 1.253<br>Psoralen 1.255 |
| $C_8H_6N_2O_2$      | 3-Phenylsydnone 1.283  | $C_{11}H_8N_2$       | Norharman 1.226   |
| $C_8H_8O$           | Acetophenone 1.2   | $C_{11}H_{10}$       | 1-Methylnaphthalene 1.223   |
| $C_8H_9ClO_2$       | 5-Chloro-1,3-dimethoxybenzene 1.74   | $C_{11}H_{11}N_3S$   | 4-(Aminomethylene)-3-methyl-1-phenyl-2-pyrazoline-5-thione 3.149  |
| $C_9H_6OS$          | Thiocoumarin 1.295   | $C_{11}H_{11}N_3Se$  | 4-(Aminomethylene)-3-methyl-1-phenyl-2-pyrazoline-5-selone 3.148  |
| $C_9H_6O_2$         | Coumarin 1.128   | $C_{11}H_{12}N_2O_4$ | $N$ -Formylkynurenone 1.76  |
| $C_9H_7N$           | Quinoline 1.268  | $C_{11}H_{13}CIS$    | 4'-Chloropivalothiophenone 1.248  |
| $C_9H_7NO$          | 4'-Cyanoacetophenone 1.3   | $C_{11}H_{13}FS$     | 4'-Fluoropivalothiophenone 1.249  |
| $C_9H_8N_2O_2$      | 3-(4-Methylphenyl)sydnone 1.281  | $C_{11}H_{14}S$      | Pivalothiophenone 1.247   |
| $C_9H_8O_2$         | 1-Phenyl-1,2-propanedione 1.251  | $C_{12}H_6Br_2S_3$   | 2,9-Dibromo- $\alpha$ -terthienyl 1.288   |
| $C_9H_9N$           | 1-Methylindole 1.217   | $C_{12}H_7BrS_3$     | 2-Bromo- $\alpha$ -terthienyl 1.286   |
| $C_9H_9NO_3S$       | 2-Methyl-4-oxo-1,2-benzothiazine 1,1-dioxide 3.24  | $C_{12}H_8Br_2N_2Pt$ | Dibromo(1,10-phenanthroline)platinum(II) 3.68   |
| $C_9H_{10}O$        | 2-Methylacetophenone biradical 1.6   | $C_{12}H_8Cl_2N_2Pt$ | Dichloro(1,10-phenanthroline)platinum(II) 3.69  |
| $C_9H_{10}O_2$      | 3'-Methoxyacetophenone 1.4<br>4'-Methoxyacetophenone 1.5   | $C_{12}H_8I_2N_2Pt$  | Diiodo(1,10-phenanthroline)platinum(II) 3.73  |
| $C_9H_{12}N_2O_5S$  | 4-Thiouridine 1.301  | $C_{12}H_8N_2$       | Phenazine 1.239   |
| $C_9H_{14}S$        | 3,3-Dimethylbicyclo[2.2.1]heptane-2-thione 1.111<br>3,5,5-Trimethyl-2-cyclohexenethione 1.132  | $C_{12}H_8N_4Pt$     | (2,2'-Bipyridine)bis(cyano)platinum(II) 3.36  |
| $C_9H_{15}CrN_6S_3$ | 1,4,7-Triazacyclonanonanetri(isothiocyanato)-chromium(III) 1.302   |                      |   |
| $C_9H_{18}S$        | Di- <i>tert</i> -butylthioketone 1.229   |                      |   |
| $C_{10}H_7Br$       | 1-Bromonaphthalene 1.222   |                      |   |
| $C_{10}H_7NO_3$     | 4-Hydroxyquinoline-2-carboxylic acid 1.269   |                      |   |

|   |                     |  |
|---|---------------------|--|
| $C_{12}H_8N_4PtS_2$   | $C_{13}H_{10}O_3$   | 4,7-Dimethylallopsoralen 1.194                                 |
| (2,2'-<br>Bipyridine)bis(thiocyanato)platinum(II)<br>3.38     |                     | 6,4-Dimethylangelicin 1.198                                    |
| $C_{12}H_8N_8Pd$  |                     | 4,5'-Dimethylangelicin 1.199                                   |
| Bis(azido)(1,10-<br>phenanthroline)palladium(II) 3.48         |                     | 4,4'-Dimethylangelicin 1.200                                   |
| $C_{12}H_8N_8Pt$  |                     | 4',5-Dimethylangelicin 1.201                                   |
| Bis(azido)(1,10-phenanthroline)platinum(II)<br>3.49           |                     | 6,4'-Dimethylangelicin 1.202                                   |
| $C_{12}H_8OS_2$   | $C_{13}H_{10}O_5$   | 5,8-Dimethoxypsoralen 1.257                                    |
| $C_{12}H_8O_3$  | $C_{13}H_{10}S_3$   | 2-Methyl- $\alpha$ -terthienyl 1.289                           |
| 4-Methylangelicin 1.203                                       | $C_{13}H_{11}NOS$   | 2-Methoxyphenothiazine 1.242                                   |
| 5-Methylangelicin 1.204                                       | $C_{13}H_{11}NS$    | 10-Methylphenothiazine 1.243                                   |
| 5'-Methylangelicin 1.205                                      | $C_{13}H_{11}N_3$   | 3,6-Diaminoacridine 1.9  |
| 4'-Methylangelicin 1.206                                      | $C_{13}H_{14}S$     | 1,1,3-Trimethyl-2-naphthalenethione 1.225                      |
| $C_{12}H_8O_4$  | $C_{13}H_{20}O$     | $\beta$ -Ionone 1.218  |
| 5-Methoxypsoralen 1.258                                       | $C_{14}H_7ClO_2$    | 1-Chloroanthraquinone 1.47                                     |
| 8-Methoxypsoralen 1.260                                       |                     | 2-Chloroanthraquinone 1.48                                     |
| $C_{12}H_8S_3$  | $C_{14}H_8Br_2$     | 9,10-Dibromoanthracene 1.17                                    |
| $C_{12}H_9NS$   | $C_{14}H_8Cl_2$     | 9,10-Dichloroanthracene 1.18                                   |
| $C_{12}H_{10}$  | $C_{14}H_8Cl_2O_2$  | 4,4'-Dichlorobenzil 1.84                                       |
| $C_{12}H_{10}N_3S^+$  | $C_{14}H_8N_4Pt$    | Dicyano(1,10-phenanthroline)palladium(II)<br>3.70              |
| $C_{12}H_{10}N_8Pd$   | $C_{14}H_8N_4PtS_2$ | (1,10-<br>Phenanthroline)bis(thiocyanato)platinum(II)<br>3.136 |
| $C_{12}H_{10}O$   |                     | 9,10-Anthraquinone 1.39  |
| $C_{12}H_{11}N_2O_3^-$  | $C_{14}H_8O_3$      | 1-Hydroxyanthraquinone 1.63                                    |
| Nalidixic acid, anion 3.134                                   |                     | 2-Hydroxyanthraquinone 1.64                                    |
| $C_{12}H_{12}N_2O_3$  | $C_{14}H_8O_4$      | 1,2-Dihydroxyanthraquinone 1.61                                |
| Nalidixic acid 3.133  |                     | 1,8-Dihydroxyanthraquinone 1.62                                |
| $C_{12}H_{12}S$   | $C_{14}H_8O_6$      | 1,4,5,8-Tetrahydroxyanthraquinone 1.66                         |
| 1,1-Dimethyl-2-naphthalenethione 1.224                        | $C_{14}H_9BrN_2O_4$ | 1,5-Diamino-2-bromo-4,8-<br>dihydroxyanthraquinone 1.54        |
| $C_{12}H_{16}OS$  |                     |  |
| 4'-Methoxypivalothiophenone 1.250                             | $C_{14}H_9Cl$       | 1-Chloroanthracene 1.14  |
| $C_{12}H_{20}S$   |                     | 9-Chloroanthracene 1.15  |
| 1,3,3,7,7-Pentamethylbicyclo[2.2.1]heptane-<br>2-thione 1.112 | $C_{14}H_9F_3O$     | 4-(Trifluoromethyl)benzophenone 1.92                           |
| $C_{13}H_7NS_3$   |                     |  |
| 2-Cyano- $\alpha$ -terthienyl 1.287                           | $C_{14}H_9NO_2$     | 1-Aminoanthraquinone 1.40                                      |
| $C_{13}H_8F_3NS$  |                     | 2-Aminoanthraquinone 1.41                                      |
| 2-(Trifluoromethyl)phenothiazine 1.244                        | $C_{14}H_9NO_3$     | 1-Amino-2-hydroxyanthraquinone 1.42                            |
| $C_{13}H_8O$  |                     | 1-Amino-4-hydroxyanthraquinone 1.43                            |
| 9-Fluorenone 1.153  | $C_{14}H_9O_3^-$    | 1,8-Dihydroxy-9-anthrone, conjugate base<br>1.69               |
| Phenalen-1-one 1.235  |                     |  |
| $C_{13}H_8O_2$  | $C_{14}H_9O_3S^-$   | 1-Anthracesulfonate ion 1.35                                   |
| Xanthone 1.316  |                     | 2-Anthracesulfonate ion 1.36                                   |
| $C_{13}H_8O_2S_3$   | $C_{14}H_{10}$      | Anthracene 1.13  |
| 2,2':5',2''-Terthiophene-5-carboxylic acid<br>1.290           |                     | Phenanthrene 1.237   |
| $C_{13}H_8O_4$  |                     |  |
| 3-Acetoallopsoralen 1.193                                     |                     |  |
| 3-Acetoangelicin 1.197  |                     |  |
| 3-Acetoisopseudopsoralen 1.209                                |                     |  |
| 3-Acetopseudoisopsoralen 1.212                                |                     |  |
| $C_{13}H_9FO$   |                     |  |
| 4-Fluorobenzophenone 1.91                                     |                     |  |
| $C_{13}H_9N$  |                     |  |
| Acridine 1.7  |                     |  |
| $C_{13}H_9NO$   |                     |  |
| 6-Aminophalenone 1.236  |                     |  |
| $C_{13}H_9NS_2$   |                     |  |
| 2,6-Bis(2-thienyl)pyridine 1.266                              |                     |  |
| $C_{13}H_{10}$  |                     |  |
| Fluorene 1.151  |                     |  |
| $C_{13}H_{10}O$   |                     |  |
| Benzophenone 1.88   |                     |  |

|                       |  |       |                         |  |
|-----------------------|--|-------|-------------------------|--|
| $C_{14}H_{10}N_2O_2$  | 1,2-Diaminoanthraquinone               | 1.49  | $C_{15}H_{15}N_3O_2$    | <i>N</i> -[4-[(2-Hydroxy-5-methylphenyl)azo]phenyl]acetamide |
|                       | 1,4-Diaminoanthraquinone               | 1.50  |                         | 3.56   |
|                       | 1,5-Diaminoanthraquinone               | 1.51  | $C_{16}H_6Br_4O_5^{2-}$ | 2,4,5,7-Tetrabromosuccinylfluorescein dianion                |
|                       | 1,8-Diaminoanthraquinone               | 1.52  |                         | 1.312  |
|                       | 2,6-Diaminoanthraquinone               | 1.53  | $C_{16}H_6I_4O_5^{2-}$  | 2,4,5,7-Tetraiodosuccinylfluorescein dianion                 |
|                       | 3,4-Diphenylsydnone                    | 1.280 |                         | 1.313  |
| $C_{14}H_{10}N_2O_4$  | 1,5-Diamino-4,8-dihydroxyanthraquinone | 1.55  | $C_{16}H_7I_3O_5^{2-}$  | 2,4,5-Triiodosuccinylfluorescein dianion                     |
|                       | 1,8-Diamino-4,5-dihydroxyanthraquinone | 1.56  |                         | 1.314  |
|                       | 2,5-Diamino-1,8-dihydroxyanthraquinone | 1.57  | $C_{16}H_8I_2O_5^{2-}$  | 4,5-Diiodosuccinylfluorescein dianion                        |
|                       | 2,7-Diamino-1,8-dihydroxyanthraquinone | 1.58  |                         | 1.311  |
| $C_{14}H_{10}O$       | Anthrone                               | 1.67  | $C_{16}H_8N_2$          | 9,10-Dicyanoanthracene                                       |
| $C_{14}H_{10}O_2$     | Benzil                                 | 1.83  | $C_{16}H_{10}$          | Fluoranthene   |
| $C_{14}H_{10}O_3$     | 1,8-Dihydroxy-9-anthrone               | 1.68  |                         | Pyrene   |
| $C_{14}H_{10}O_4$     | 5'-Aceto-8-methylpsoralen              | 1.211 |                         | Pyrene, excimer  |
| $C_{14}H_{10}O_5$     | 3-Carbethoxypseudopsoralen             | 1.254 | $C_{16}H_{10}AlN_2O_2$  | Aluminum(III) 1-(2-hydroxyphenylazo)-2-naphtholate           |
|                       | 3-Carbethoxypsoralen                   | 1.256 |                         | 3.122  |
| $C_{14}H_{10}S$       | 2-(1-Naphthyl)thiophene                | 1.297 | $C_{16}H_{10}CrN_2O_2$  | Chromium(III) 1-(2-hydroxyphenylazo)-2-naphtholate           |
|                       | 2-(2-Naphthyl)thiophene                | 1.298 |                         | 3.123  |
| $C_{14}H_{10}S_2$     | 2,2'-(1,3-Phenylene)bisthiophene       | 1.299 | $C_{16}H_{10}CuN_2O_2$  | Copper(II) 1-(2-hydroxyphenylazo)-2-naphtholate              |
|                       | 2,2'-(1,4-Phenylene)bisthiophene       | 1.300 |                         | 3.126  |
| $C_{14}H_{11}NOS$     | 2-Acetylphenothiazine                  | 1.241 | $C_{16}H_{10}FeN_2O_2$  | Iron(III) 1-(2-hydroxyphenylazo)-2-naphtholate               |
| $C_{14}H_{11}NS$      | 10-Methyl-9-acridinethione             | 1.8   |                         | 3.127  |
| $C_{14}H_{12}$        | (E)-Stilbene                           | 1.279 | $C_{16}H_{10}N_2NiO_2$  | Nickel(II) 1-(2-hydroxyphenylazo)-2-naphtholate              |
| $C_{14}H_{12}N_4O_2$  | 1,4,5,8-Tetraaminoanthraquinone        | 1.65  |                         | 3.128  |
| $C_{14}H_{12}O_3$     | 4,7,5'-Trimethylallopsoralen           | 1.195 | $C_{16}H_{10}N_2O_2Zn$  | Zinc(II) 1-(2-hydroxyphenylazo)-2-naphtholate                |
|                       | 4,7,4'-Trimethylallopsoralen           | 1.196 |                         | 3.129  |
|                       | 6,4,4'-Trimethylangelicin              | 1.207 | $C_{16}H_{10}S_4$       | $\alpha$ -Quaterthienyl                                      |
|                       | 4,5',8-Trimethylpsoralen               | 1.261 | $C_{16}H_{11}NS$        | Benzo[a]phenothiazine  |
| $C_{14}H_{14}N_3^+$   | 3,6-Diamino-10-methylacridinium        | 1.10  |                         | 1.93   |
| $C_{14}H_{14}O_3$     | Naproxen                               | 3.113 |                         | Benzo[b]phenothiazine  |
| $C_{14}H_{17}NO_2$    | 7-(Diethylamino)-4-methylcoumarin      | 1.129 |                         | 1.94   |
| $C_{15}H_9N$          | 9-Cyanoanthracene                      | 1.16  |                         | Benzo[c]phenothiazine  |
| $C_{15}H_{10}O_2$     | Flavone                                | 1.98  | $C_{16}H_{11}N_3O_3$    | 1-(4-Nitrophenylazo)-2-naphthol                              |
| $C_{15}H_{10}O_3$     | 3-Hydroxyflavone                       | 1.97  | $C_{16}H_{12}$          | 2-Vinylanthracene  |
| $C_{15}H_{11}NO_2$    | 1-Amino-2-methylanthraquinone          | 1.46  | $C_{16}H_{12}ClNO_3$    | Benoaprofen  |
| $C_{15}H_{12}$        | 9-Methylanthracene                     | 1.26  |                         | 3.31   |
| $C_{15}H_{12}N_2O_2$  | 3-(4-Methylphenyl)-4-phenylsydnone     | 1.282 | $C_{16}H_{12}S$         | 2,5-Diphenylthiophene  |
| $C_{15}H_{12}N_2O_3$  | 1,4-Diamino-2-methoxyanthraquinone     | 1.59  | $C_{16}H_{14}$          | 9,10-Dimethylanthracene                                      |
| $C_{15}H_{12}O_4$     | 5'-Aceto-4,8-dimethylpsoralen          | 1.210 | $C_{16}H_{14}FN_3O$     | Afloqualone  |
| $C_{15}H_{13}N_3O_4S$ | Piroxicam                              | 3.23  |                         | 3.163  |
| $C_{15}H_{14}O_2S$    | 4,4'-Dimethoxythiobenzophenone         | 1.293 | $C_{16}H_{14}N_2^{2+}$  | <i>N,N'</i> -Dimethyl-2,7-diazapyprene                       |
| $C_{15}H_{14}O_3$     | 4,4'-Dimethoxybenzophenone             | 1.90  | $C_{16}H_{14}O_4$       | 4,4'-Dimethoxybenzil   |
|                       |  |       | $C_{16}H_{15}N_3O_2$    | 1-(Phenylazo)-1-(phenylaminocarbonyl)-2-propanone            |
|                       |  |       |                         | 3.62   |

|                          |  |       |                                |   |
|--------------------------|--|-------|--------------------------------|---|
| $C_{16}H_{17}NO_2$       | 2,3,6,7-Tetrahydro-9-methyl[1]benzopyran[6,7,8-ij]quinolizine-1-one            | 1.99  | $C_{18}H_{14}N_3O_6S^-$        | 5-Methoxy-4-[2-(methylsulfonyl)-4-nitrophenyl]azo-1-naphthoxide ion           |
| $C_{16}H_{18}N_3S^+$     | Methylene Blue cation  | 1.245 |                                | 3.121   |
| $C_{17}H_{10}O$          | 1-Pyrenecarboxaldehyde   | 1.265 | $C_{18}H_{16}$                 | 1,6-Diphenyl-1,3,5-hexatriene   |
| $C_{17}H_{13}N_3O_3$     | 1-(4-Methyl-2-nitrophenylazo)-2-naphthol                                       | 3.130 | $C_{18}H_{18}$                 | 9- <i>tert</i> -Butylanthracene   |
| $C_{17}H_{14}$           | (E)-2-(1-Propenyl)anthracene   | 1.32  | $C_{18}H_{18}N_4O$             | 4-(4'-Dimethylaminophenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one           |
| $C_{17}H_{15}N_5$        | 1,3-Dimethylpyrazolo[1',2':2,3][1,2,3]-triazolo[4,5- <i>a</i> ]phenazin-4-i um | 3.158 |                                | 3.157   |
| $C_{17}H_{17}N_3O_2$     | 1-(4-Methylphenylazo)-1-(phenylaminocarbonyl)-2-propanone                      | 3.61  | $C_{19}H_7Cl_4I_4O_5^-$        | 9-(2,3,4,5-Tetrachlorophenyl)-6-hydroxy-2,4,5,7-tetraiodoxanthen-3-one, anion |
| $C_{17}H_{19}ClN_2S$     | Chlorpromazine   | 3.142 |                                | 1.315   |
| $C_{17}H_{20}N_2O$       | 4,4'-Bis(dimethylamino)benzophenone  | 1.89  | $C_{19}H_{12}N_2O_2PdS$        | Phenanthroline(thiosalicylato)palladium(II)                                   |
| $C_{17}H_{20}N_4O_6$     | Riboflavin e   | 1.274 |                                | 3.139   |
| $C_{17}H_{21}N_4O_9P$    | Flavine mononucleotide   | 1.275 | $C_{19}H_{13}O_2S^-$           | 9-(Phenylsulfonyl)fluorene anion  |
| $C_{17}H_{24}O$          | (E,E,E)-5-Methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6-heptatrienal      | 1.214 | $C_{19}H_{14}N_2PdS_2$         | 3,4-Dimercaptotoluene(1,10-phenanthroline)palladium(II)                       |
| $C_{18}H_6N_4$           | 2,6,9,10-Tetracyanoanthracene  | 1.33  |                                | 3.74  |
| $C_{18}H_{11}Br$         | 2-Bromochrysene  | 1.125 | $C_{19}H_{14}S$                | 4-Phenylthiobenzophenone  |
| $C_{18}H_{11}Cl$         | 2-Chlorochrysene   | 1.126 | $C_{19}H_{17}N_3O$             | 4-(Dicyanomethylene)-2-methyl-6-( <i>p</i> -dimethylaminostyryl)pyran         |
| $C_{18}H_{12}$           | Benz[ <i>a</i> ]anthracene   | 1.72  |                                | 3.146   |
|                          | Chrysene   | 1.124 | $C_{19}H_{18}N_2O_{11}S_3.2Na$ | Remazol Red B   |
|                          | Tetracene  | 1.291 |                                | 3.118   |
|                          | Triphenylene   | 1.304 | $C_{19}H_{18}N_4O_{11}.2Na$    | Active Yellow 2KT   |
| $C_{18}H_{12}N_2O_2Pd$   | Catechol(1,10-phenanthroline)palladium(II)                                     | 3.53  | $C_{19}H_{18}O_8$              | Daunomycinone   |
| $C_{18}H_{12}N_2O_2Pt$   | Catechol(1,10-phenanthroline)platinum(II)                                      | 3.54  | $C_{20}H_2Br_4Cl_4O_5^{2-}$    | Tetrachloroeosin dianion  |
| $C_{18}H_{12}N_8Pd$      | Bis(azido)(2,2'-biquinoline)palladium(II)                                      | 3.43  | $C_{20}H_2Cl_4I_4O_5^{2-}$     | Rose Bengal dianion   |
| $C_{18}H_{12}N_8Pt$      | Bis(azido)(2,2'-biquinoline)platinum(II)                                       | 3.44  |                                | 1.169   |
| $C_{18}H_{12}O_2$        | 2,6-Diphenyl-1,4-benzoquinone  | 1.100 | $C_{20}H_4Cl_4I_4O_5$          | Rose Bengal lactone   |
|                          | 2,6-Diphenyl-1,4-benzoquinone/Triphenylamine                                   | 1.101 |                                | 1.168   |
| $C_{18}H_{14}$           | <i>p</i> -Terphenyl  | 1.284 | $C_{20}H_6Br_2N_2O_9^{2-}$     | Eosin B dianion   |
| $C_{18}H_{14}Br_2N_3O^+$ | 5-Amino-6,8-dibromo-9-ethylaminobenzo[ <i>a</i> ]phenoxazinium                 | 3.16  | $C_{20}H_6Br_4O_5^{2-}$        | Eosin dianion   |
| $C_{18}H_{14}I_2N_3O^+$  | 5-Amino-9-ethylamino-6,8-diiodobenzo[ <i>a</i> ]phenoxazinium                  | 3.19  | $C_{20}H_6Cl_4O_5^{2-}$        | 2',4',5',7'-Tetrachlorofluorescein dianion                                    |
|                          |  |       |                                | 1.167   |
|                          |  |       | $C_{20}H_6I_4O_5^{2-}$         | Erythrosin dianion  |
|                          |  |       | $C_{20}H_7Br_3O_5^{2-}$        | Tribromofluorescein dianion   |
|                          |  |       | $C_{20}H_8Br_2O_5^{2-}$        | Dibromofluorescein dianion  |
|                          |  |       | $C_{20}H_8Cl_2O_5^{2-}$        | 2',7'-Dichlorofluorescein dianion   |
|                          |  |       |                                | 1.158   |
|                          |  |       |                                | 4',5'-Dichlorofluorescein dianion   |
|                          |  |       |                                | 1.159   |

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| $C_{20}H_8I_2O_5^{2-}$  | Diiodofluorescein dianion   | 1.160 | $C_{20}H_{20}N_3O^+$   | 5-Amino-9-diethylaminobenzo[ <i>a</i> ]phenoxazinium   |
| $C_{20}H_9BrClNO_2S$    | 5-Bromo-2-(9-chloro-3-oxonaphtho-[1,2- <i>b</i> ]thien-2-ylidene)-4-methyl-1,2-dihydroindol-3-one           | 3.102 | $C_{20}H_{20}N_3S^+$   | 3.17   |
| $C_{20}H_{10}O_5^{2-}$  | Fluorescein dianion   | 1.154 | $C_{20}H_{20}N_3S^+$   | 5-Amino-9-diethylaminobenzo[ <i>a</i> ]phenothiazinium   |
| $C_{20}H_{12}$          | Perylene  | 1.233 | $C_{20}H_{21}N_7O_7$   | 3.12   |
| $C_{20}H_{12}D_2N_4$    | Porphine-21,23- <i>d</i> <sub>2</sub>   | 2.47  | $N$ -[5-[(2-Cyanoethyl)(2-hydroxyethyl)amino]-2-[(2,4-dinitrophenyl)azo]-4-methoxyphenyl]acetamide | 3.60   |
| $C_{20}H_{13}NO_4$      | 1-Amino-4-hydroxy-2-phenoxyanthraquinone  | 1.44  | $C_{20}H_{22}N_2S$   | Mequitazine  |
| $C_{20}H_{14}$          | 9-Phenylanthracene  | 1.29  | $C_{20}H_{22}N_4O$   | 4-(4'-Diethylaminophenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one   |
| $C_{20}H_{14}N_2O_2Pd$  | 2,2'-Bipyridine(2,3-naphthalenediolato)palladium(II)  | 3.39  | $C_{20}H_{22}O_2$  | 2,2',4,4',6,6'-Hexamethylbenzil  |
| $C_{20}H_{14}N_2O_2Pt$  | 2,2'-Bipyridine(2,3-naphthalenediolato)platinum(II)   | 3.40  | $C_{20}H_{28}O$  | 13-( <i>Z</i> )-Retinal  |
| $C_{20}H_{14}N_4$       | Porphine  | 2.46  | $C_{20}H_{30}O$  | ( <i>all-E</i> )-Retinal   |
|                         | Porphycene  | 2.211 | $C_{21}H_5Cl_4I_4O_5^-$  | Rose Bengal monoanion, methyl ester  |
| $C_{20}H_{14}O$         | 1,3-Diphenylisobenzofuran   | 1.219 |  | 1.188  |
| $C_{20}H_{16}$          | 9,10-Dimethylbenz[ <i>a</i> ]anthracene   | 1.73  | $C_{21}H_6Cl_4I_4O_5^-$  | Rose Bengal, methyl ester  |
| $C_{20}H_{18}$          | 1,8-Diphenyl-1,3,5,7-octatetraene   | 1.227 | $C_{21}H_9Br_4O_5^-$   | Eosin monoanion, methyl ester  |
| $C_{20}H_{18}I_2N_3O^+$ | 5-Amino-9-diethylamino-2,6-diiodobenzo[ <i>a</i> ]phenoxazinium   | 3.18  | $C_{21}H_{10}Br_4O_5^-$  | 1.165  |
| $C_{20}H_{19}BrN_3O^+$  | 5-Amino-6-bromo-9-diethylaminobenzo[ <i>a</i> ]phenoxazinium  | 3.15  | $C_{21}H_{13}CoN_5O_3$   | Eosin, methyl ester  |
| $C_{20}H_{19}IN_3O^+$   | 5-Amino-9-diethylamino-2-iodobenzo[ <i>a</i> ]phenoxazinium   | 3.20  |  | 3.91   |
|                         | 5-Amino-9-diethylamino-6-iodobenzo[ <i>a</i> ]phenoxazinium   | 3.21  |  | Cobalt(III) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate  |
| $C_{20}H_{19}IN_3S^+$   | 5-Amino-9-diethylamino-6-iodobenzo[ <i>a</i> ]phenothiazinium   | 3.13  |  | 3.92   |
| $C_{20}H_{19}N_4^+$     | Safranine cation  | 3.183 | $C_{21}H_{13}CuN_5O_3$   | Copper(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate   |
| $C_{20}H_{20}$          | ( <i>E</i> )-2-(3,3-Dimethyl-1-butenyl)anthracene   | 1.22  |  | 3.93   |
|                         | ( <i>Z</i> )-2-(3,3-Dimethyl-1-butenyl)anthracene   | 1.23  | $C_{21}H_{13}N_5NiO_3$   | Nickel(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate   |
| $C_{20}H_{20}BrN_7O_7$  | $N$ -[2-[(2-Bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide  | 3.58  |  | 3.94   |
| $C_{20}H_{20}ClN_7O_7$  | $N$ -[2-[(2-Chloro-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide | 3.59  | $C_{21}H_{14}O_2$  | 2,3-Diphenylchromone   |
|                         |   |       | $C_{21}H_{14}O_6S_2^{2-}$  | 1,1'-Methylenebis(6-naphthalenesulfonate ion)  |
|                         |   |       | $C_{21}H_{15}BrN_2O_5S.Na$   | 3.119  |
|                         |   |       | $C_{21}H_{20}BrN_7O_5$   | Acid Pure Sky Blue   |
|                         |   |       |  | 3.7  |
|                         |   |       |  | $N$ -[2-[(2-Bromo-6-cyano-4-nitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide |
|                         |   |       |  | 3.57   |
|                         |   |       | $C_{21}H_{24}N_4O$   | 4-(4'-Diethylamino-2'-methylphenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one                                   |
|                         |   |       |  | 3.154  |
|                         |   |       | $C_{22}H_8Cl_4I_4O_5$  | Rose Bengal, ethyl ester   |
|                         |   |       |  | 1.182  |
|                         |   |       |  | <i>O</i> -Methyl Rose Bengal methyl ester  |
|                         |   |       |  | 1.186  |

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|---|--|-------|--|--|-------|
| C <sub>22</sub> H <sub>12</sub>   | Dibenzo[def,mno]chrysene   | 1.138 | C <sub>23</sub> H <sub>27</sub> N <sub>5</sub> O <sub>2</sub>                        | 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(3-methylphenyl)pyrazol-3-one  | 3.153 |
| C <sub>22</sub> H <sub>14</sub>   | Dibenz[a,h]anthracene  | 1.137 | C <sub>23</sub> H <sub>27</sub> N <sub>5</sub> O <sub>3</sub>                        | 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(3-methoxyphenyl)pyrazol-3-one | 3.152 |
| C <sub>22</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> Pd                          | 1,10-Phenanthroline(2,3-naphthalenediolato)platinum(II)  | 3.137 | C <sub>24</sub> H <sub>10</sub> Br <sub>2</sub> O <sub>2</sub>                       | 4,9-Dibromo-2,3:7,8-dibenzopyrene-1,6-dione  | 3.66  |
| C <sub>22</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> Pt                          | 1,10-Phenanthroline(2,3-naphthalenediolato)platinum(II)  | 3.138 | C <sub>24</sub> H <sub>10</sub> Cl <sub>2</sub> O <sub>2</sub>                       | 4,9-Dichloro-2,3:7,8-dibenzopyrene-1,6-dione   | 3.67  |
| C <sub>22</sub> H <sub>16</sub>   | (Z)-2-(2-Phenylethenyl)anthracene  | 1.30  | C <sub>24</sub> H <sub>10</sub> Cl <sub>4</sub> I <sub>4</sub> O <sub>6</sub>        | 6-O-Acetyl Rose Bengal ethyl ester   | 1.170 |
|   | (E)-2-(2-Phenylethenyl)anthracene  | 1.31  | C <sub>24</sub> H <sub>12</sub>  | Coronene   | 1.127 |
| C <sub>22</sub> H <sub>16</sub> N <sub>2</sub> O <sub>11</sub> S <sub>3</sub>             | Remazol Brilliant Blue R   | 3.6   | C <sub>24</sub> H <sub>12</sub> Br <sub>2</sub> O <sub>2</sub>                       | 4,10-Dibromoanthanthrone   | 3.64  |
| C <sub>22</sub> H <sub>16</sub> N <sub>6</sub> Ru   | Bis(2,2'-bipyridine)bis(cyano)ruthenium(II)  | 1.116 | C <sub>24</sub> H <sub>12</sub> O <sub>2</sub>                                       | 2,3:7,8-Dibenzopyrene-1,6-dione  | 3.65  |
| C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>2</sub> Pd                          | 4-tert-Butylcatechol(1,10-phenanthroline)palladium(II)   | 3.50  | C <sub>24</sub> H <sub>12</sub> O <sub>2</sub> S <sub>2</sub>                        | (E)-Perinaphthothioindigo  | 3.132 |
| C <sub>22</sub> H <sub>22</sub> Cl <sub>3</sub> N <sub>5</sub> O <sub>2</sub>             | 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(2,4,6-trichlorophenyl)pyrazol-3-one     | 3.155 | C <sub>24</sub> H <sub>12</sub> S  | Diacenaphtho[1,2-b:2',1'-d]thiophene   | 1.135 |
| C <sub>22</sub> H <sub>24</sub> BrN <sub>5</sub> O <sub>2</sub>                           | 2,4-Dihydro-2-(4-bromophenyl)-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamylpyrazol-3-one             | 3.150 | C <sub>24</sub> H <sub>16</sub> N <sub>8</sub> Pd                                    | Bis(azido)(4,7-diphenyl-1,10-phenanthroline)palladium(II)  | 3.46  |
| C <sub>22</sub> H <sub>24</sub> ClN <sub>5</sub> O <sub>2</sub>                           | 2,4-Dihydro-2-(4-chlorophenyl)-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamylpyrazol-3-one            | 3.151 | C <sub>24</sub> H <sub>16</sub> N <sub>8</sub> Pt                                    | Bis(azido)(4,7-diphenyl-1,10-phenanthroline)platinum(II)   | 3.47  |
| C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>8</sub>                             | Tetracycline   | 3.108 | C <sub>24</sub> H <sub>18</sub>  | 1,3,5-Triphenylbenzene   | 1.75  |
| C <sub>22</sub> H <sub>30</sub> O   | $\beta$ -apo-14'-Carotenal   | 1.122 | C <sub>24</sub> H <sub>19</sub> N <sub>3</sub> O <sub>2</sub>                        | 1-(4-Methylphenylazo)-3-(phenylaminocarbonyl)-2-naphthol   | 3.115 |
| C <sub>23</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>                             | 3-Methyl-6-(phenylamino)dibenz[f,i,j]isoquinoline-2,7-dione  | 3.63  | C <sub>24</sub> H <sub>32</sub> NO <sub>3</sub> S <sub>2</sub> <sup>-</sup>          | 12-(10'-Phenothiazinyl)dodecyl-1-sulfonate ion   | 3.143 |
| C <sub>23</sub> H <sub>18</sub> CoN <sub>4</sub> O <sub>2</sub>                           | Cobalt(II) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate   | 3.85  | C <sub>25</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>                        | 4-Benzoylbenzimidazo[2,10a]benz[de]isoquinolin-7-one   | 3.10  |
|   | Cobalt(III) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate  | 3.86  | C <sub>25</sub> H <sub>18</sub> ClN <sub>7</sub> O <sub>10</sub> S <sub>3</sub> .3Na | Procion Red H-3B   | 3.116 |
| C <sub>23</sub> H <sub>18</sub> CrN <sub>4</sub> O <sub>2</sub>                           | Chromium(III) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate  | 3.87  | C <sub>25</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub>                        | 1-(4-Aminocarbonylphenylazo)-3-(2-methoxyphenylaminocarbonyl)-2-naphthol                             | 3.114 |
| C <sub>23</sub> H <sub>18</sub> CuN <sub>4</sub> O <sub>2</sub>                           | Copper(II) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate   | 3.88  | C <sub>25</sub> H <sub>25</sub> IN <sub>2</sub>                                      | 1,1'-Diethyl-4,4'-carbocyanine iodide  | 3.52  |
| C <sub>23</sub> H <sub>18</sub> H <sub>5</sub> O <sub>9</sub> S <sub>3</sub> <sup>-</sup> | N-[5-Hydroxy-8-[[2-(methylsulfonyl)-4-nitrophenyl]azo]-1-naphthalenyl-1,3-benzenedisulfonamide, conjugate base | 3.120 | C <sub>25</sub> H <sub>25</sub> IN <sub>2</sub> O <sub>2</sub>                       | 3,3'-Diethyl-2,2'-oxatricarbocyanine iodide  | 3.135 |
| C <sub>23</sub> H <sub>25</sub> N <sub>2</sub> <sup>+</sup>                               | Malachite Green cation   | 3.103 | C <sub>25</sub> H <sub>25</sub> IN <sub>2</sub> S <sub>2</sub>                       | 3,3'-Diethyl-2,2'-thiatricarbocyanine iodide   | 3.194 |
|   |  |       | C <sub>25</sub> H <sub>28</sub> N <sub>4</sub> O <sub>10</sub>                       | Riboflavin-2',3',4',5'-tetraacetate  | 1.276 |
|   |  |       | C <sub>26</sub> H <sub>14</sub>  | Rubicene   | 1.277 |
|   |  |       | C <sub>26</sub> H <sub>14</sub> O <sub>2</sub>                                       | Anthra[1,9-bc:4,10-b'c']dichromene   | 1.37  |
|   |  |       |  | Benzo[1,2,3-kl:4,5,6-k'l']dixanthene   | 1.87  |

|                            |  |       |                           |   |       |
|----------------------------|--|-------|---------------------------|---|-------|
| $C_{26}H_{16}N_6Ru$        | Dicyanobis(1,10-phenanthroline)ruthenium(II)   | 1.140 | $C_{27}H_{28}N_2O_9$      | 5-Iminodaunomycin   | 3.112 |
| $C_{26}H_{17}ClN_7O_9Na$   | Cibacron Rubine 4G-P   | 3.117 | $C_{27}H_{29}NO_{10}$     | Daunomycin  | 3.109 |
| $C_{26}H_{18}$             | 9,10-Diphenylanthracene<br>(E)-2-[2-(2-Naphthyl)ethenyl]anthracene<br>1.27   | 1.25  | $C_{27}H_{29}NO_{11}$     | Adriamycin  | 3.111 |
|                            | (Z)-2-[2-(2-Naphthyl)ethenyl]anthracene<br>1.28  | 1.28  | $C_{27}H_{41}Te_2^+$      | 2,6-Bis(1,1-dimethylethyl)-4-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]ethyltelluropyrylium             | 3.192 |
| $C_{26}H_{18}N_2^{2+}$     | $N,N'$ -Dimethylanthra[2,1,0-def:6,5,10-d'e'f']diisoquinoline  | 1.38  | $C_{27}H_{44}O$           | 7-Dehydrocholesterol  | 1.134 |
| $C_{26}H_{18}N_2O_6S$      | 1-Amino-4-hydroxy-2-[4-(phenylamino-sulfonyl)phenoxy]anthraquinone   | 1.45  | $C_{28}H_{14}N_2O_2S_2$   | 1,8-Diphenylanthra[2,1-d:6,5-d']bisthiazole-6,12-dione  | 3.5   |
| $C_{26}H_{19}N_3O_5S$      | 1,4-Diamino-[4-(phenylamino-sulfonyl)phenoxy]anthraquinone   | 1.60  | $C_{28}H_{14}O_2$         | Heterocoerdianthrone  | 1.215 |
| $C_{26}H_{25}ClIN_2S$      | 6-Chloro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate  | 3.26  | $C_{28}H_{16}$            | Helianthrene  | 1.213 |
| $C_{26}H_{25}FIN_2S$       | 6-Fluoro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate  | 3.28  | $C_{28}H_{18}N_2O_2Pd$    | 2,2'-Biquinoline(2,3-naphthalenediolato)palladium(II)   | 3.41  |
| $C_{26}H_{27}IN_2S$        | 3-Methyl-2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]benzothiazolium, iodide                             | 3.30  | $C_{28}H_{18}N_2O_2Pt$    | 2,2'-Biquinoline(2,3-naphthalenediolato)platinum(II)  | 3.42  |
| $C_{26}H_{33}N_3NaO_6S_2$  | Merocyanine 540  | 3.32  | $C_{28}H_{22}O_2$         | 1,4-Dimethoxy-9,10-diphenylanthracene   | 1.20  |
| $C_{27}H_9Cl_4I_4O_5^-$    | Rose Bengal monoanion, benzyl ester  | 1.172 | $C_{28}H_{23}Cl_4I_4NO_5$ | Rose Bengal, ethyl ester, triethylammonium salt   | 1.183 |
| $C_{27}H_{10}Cl_4I_4O_5^-$ | Rose Bengal, benzyl ester  | 1.171 | $C_{28}H_{28}D_2N_4$      | 2,3,12,13-Tetraethylporphyrin-d <sub>2</sub>  | 2.60  |
| $C_{27}H_{13}Br_4O_5^-$    | Eosin monoanion, benzyl ester  | 1.162 | $C_{28}H_{30}N_4$         | 2,3,7,8-Tetraethylporphyrin   | 2.91  |
| $C_{27}H_{26}N_3O^+$       | 5-Benzylamino-9-diethylaminobenzo[a]phenoxazinium  | 3.22  |                           | 2,3,12,13-Tetraethylporphyrin   | 2.92  |
| $C_{27}H_{26}N_3S^+$       | 5-Benzylamino-9-diethylaminobenzo[a]phenothiazinium  | 3.14  |                           | 3,7,12,18-Tetramethyl-2,8-diethylporphyrin  | 2.135 |
| $C_{27}H_{26}O_9$          | Gilvocarcin V  | 3.11  | $C_{28}H_{31}N_2O_3^+$    | Rhodamine B cation  | 3.165 |
| $C_{27}H_{28}IN_2OS$       | 6-Methoxy-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate | 3.29  |                           | Rhodamine 6G cation   | 3.166 |
| $C_{27}H_{28}IN_2S$        | 3,6-Dimethyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate       | 3.27  | $C_{28}H_{43}Te_2^+$      | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]ethyl]telluropyrylium         | 3.191 |
|                            |  |       | $C_{28}H_{44}O$           | Ergosterol  | 1.142 |
|                            |  |       | $C_{29}H_{19}ClN_7O_5Na$  | Active Brilliant Sky Blue 2KT   | 3.8   |
|                            |  |       | $C_{29}H_{26}O_{10}$      | Cercosporin   | 1.234 |
|                            |  |       | $C_{29}H_{31}Cl_2IN_2$    | 5,5'-Dichloro-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide  | 3.198 |
|                            |  |       | $C_{29}H_{31}F_2IN_2$     | 5,5'-Difluoro-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide  | 3.199 |
|                            |  |       | $C_{29}H_{32}BBrF_4N_2$   | 2-[7-(4-Bromo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate | 3.95  |

|                         |  |       |                             |   |       |
|-------------------------|--|-------|-----------------------------|---|-------|
| $C_{29}H_{32}BClF_4N_2$ | 2-[7-(4-Chloro-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate | 3.96  | $C_{29}H_{45}O_2SeTe^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]-selenopyrylium | 3.184 |
| $C_{29}H_{32}BF_4IN_2$  | 2-[7-(4-Iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate   | 3.98  | $C_{30}H_{15}Cl_4I_4O_5^-$  | Rose Bengal monoanion, <i>p</i> -isopropylbenzyl ester  | 1.185 |
| $C_{29}H_{32}I_2N_2$    | 2-[7-(4-Iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, iodide              | 3.97  | $C_{30}H_{16}$              | Pyranthrene   | 1.262 |
| $C_{29}H_{33}ClN_2O_4$  | 1,1',3,3,3',3'-Hexamethyltricarbocyanine, perchlorate  | 3.203 | $C_{30}H_{16}Cl_4I_4O_5$    | Rose Bengal, <i>p</i> -isopropylbenzyl ester  | 1.184 |
| $C_{29}H_{33}FN_2$      | 1,1',3,3,3',3'-Hexamethyltricarbocyanine, fluoride   | 3.201 | $C_{30}H_{16}O_8$           | Hypericin   | 1.238 |
| $C_{29}H_{33}IN_2$      | 1,1',3,3,3',3'-Hexamethyltricarbocyanine, iodide   | 3.202 | $C_{30}H_{19}Br_4O_5^-$     | Eosin monoanion, <i>p</i> -isopropylbenzyl ester  | 1.163 |
| $C_{29}H_{43}OS^+$      | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)thiapyran-4-ylidene]-3-propenyl]pyrylium              | 3.161 | $C_{30}H_{20}O_3$           | 11,12-Dibenzoyl-9,10-dihydro-9-hydroxy-9,10-ethenoanthracene  | 1.145 |
| $C_{29}H_{43}OSe^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]pyrylium            | 3.159 | $C_{30}H_{24}IrN_6^{3+}$    | Tris(2,2'-bipyridine)iridium(III) ion   | 1.305 |
| $C_{29}H_{43}OTe^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]pyrylium           | 3.160 | $C_{30}H_{24}N_6Ru^{2+}$    | Tris(2,2'-bipyridine)ruthenium(II) ion  | 1.306 |
| $C_{29}H_{43}O_2^+$     | 4,4'-(1,3-Propenyl)bis[2,6-di(1,1-dimethylethyl)pyrylium   | 3.162 | $C_{30}H_{30}N_4O_4$        | Deuteroporphyrin IX   | 2.197 |
| $C_{29}H_{43}SSe^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]thiopyrylium        | 3.195 | $C_{30}H_{45}Se_2^+$        | 2,6-Bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-4-(2-butenyl)]selenopyrylium              | 3.185 |
| $C_{29}H_{43}STe^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]thiopyrylium       | 3.196 | $C_{31}H_{19}NO_2$          | 11,12-Dibenzoyl-9,10-dihydro-9,10-ethenoanthracene-9-carbonitrile   | 1.148 |
| $C_{29}H_{43}S_2^+$     | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)thiopyran-4-ylidene]-3-propenyl]thiopyrylium          | 3.197 | $C_{31}H_{20}O_3$           | 11,12-Dibenzoyl-9,10-dihydro-9,10-ethenoanthracene-9-carboxaldehyde   | 1.149 |
| $C_{29}H_{43}SeTe^+$    | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]selenopyrylium     | 3.188 | $C_{31}H_{22}O_3$           | 11,12-Dibenzoyl-9,10-dihydro-9-methoxy-9,10-ethenoanthracene  | 1.146 |
| $C_{29}H_{43}Se_2^+$    | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]selenopyrylium      | 3.187 | $C_{31}H_{28}N_4O_3$        | Deuteroverdin methyl ester  | 2.228 |
| $C_{29}H_{43}Te_2^+$    | 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]telluropyrylium    | 3.193 | $C_{31}H_{37}IN_2$          | 1,1',3,3,3',3'-Octamethyltricarbocyanine, iodide  | 3.204 |
|                         |  |       | $C_{31}H_{37}IN_2O_2$       | 5,5'-Dimethoxy-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide   | 3.200 |
|                         |  |       | $C_{31}H_{47}Se_2^+$        | 2,6-Bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-4-(2-pentenyl)]selenopyrylium             | 3.186 |
|                         |  |       | $C_{32}H_{12}AlClN_8O_9S_3$ | Chloroaluminum(III) sulfophthalocyanine   | 2.29  |
|                         |  |       | $C_{32}H_{12}AlN_8O_9S_3$   | Aluminum(III) sulfophthalocyanine   | 2.30  |
|                         |  |       | $C_{32}H_{12}ClGaN_8O_9S_3$ | Chlorogallium(III) sulfophthalocyanine  | 2.36  |

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| $C_{32}H_{12}ClGaN_8O_{12}S_4^{4-}$                      |   |       |
| Chlorogallium(III) tetrasulfophthalocyanine              |   |       |
| 2.35   |   |       |
| $C_{32}H_{12}CoN_8O_9S_3$                                |   |       |
| Cobalt(II) sulfophthalocyanine                           | 2.32  |       |
| $C_{32}H_{12}CuN_8O_9S_3$                                |   |       |
| Copper(II) sulfophthalocyanine                           | 2.33  |       |
| $C_{32}H_{12}FeN_8O_9S_3$                                |   |       |
| Iron(II) sulfophthalocyanine                             | 2.34  |       |
| $C_{32}H_{12}N_8O_9S_3$                                  |   |       |
| Sulfophthalocyanine                                      | 2.27  |       |
| $C_{32}H_{12}N_8O_{10}S_3V$                              |   |       |
| Sulfophthalocyaninatooxovanadate(IV) ion                 |   |       |
| 2.37   |   |       |
| $C_{32}H_{13}AlClN_8O_9S_3^{3-}$                         |   |       |
| Chloroaluminum(III) trisulfophthalocyanine               |   |       |
| 2.28   |   |       |
| $C_{32}H_{13}N_8O_9S_3Zn^{3-}$                           |   |       |
| Zinc(II) trisulfophthalocyanine                          | 2.38  |       |
| $C_{32}H_{16}MgN_8$                                      |   |       |
| Magnesium(II) phthalocyanine                             | 2.24  |       |
| $C_{32}H_{18}O_2$  | 8,16-Pyranthredione   | 3.147 |
| $C_{32}H_{20}CoN_4O_4$                                   |   |       |
| Cobalt(II) bis[1-(2-hydroxyphenylazo)-2-naphtholate]     | 3.124   |       |
| Cobalt(III) bis[1-(2-hydroxyphenylazo)-2-naphtholate]    | 3.125   |       |
| $C_{32}H_{22}O_4$  | 9-Acetoxy-11,12-dibenzoyl-9,10-dihydro-9,10-ethenoanthracene  | 1.143 |
| $C_{32}H_{24}O_2$  | 11,12-Dibenzoyl-9-ethyl-9,10-dihydro-9,10-ethenoanthracene  | 1.147 |
| $C_{32}H_{24}O_4$  | 11,12-Dibenzoyl-9,10-dihydro-9,10-dimethoxy-9,10-ethenoanthracene   | 1.144 |
| $C_{32}H_{30}N_4OZn$                                     |   |       |
| Zinc methyl pyoverdin                                    | 2.226   |       |
| $C_{32}H_{32}D_2N_4O_4$                                  |   |       |
| Deuteroporphyrin- <i>d</i> <sub>2</sub> , dimethyl ester | 2.199   |       |
| $C_{32}H_{33}CdClN_6O_3$                                 |   |       |
| Cadmium(II) chlorotexaphyrin nitrate                     |   |       |
| 2.219  |   |       |
| $C_{32}H_{33}Cl_2N_5Zn$                                  |   |       |
| Zinc(II) chlorotexaphyrin chloride                       | 2.224   |       |
| $C_{32}H_{34}CdN_6O_3$                                   |   |       |
| Cadmium(II) texaphyrin nitrate                           | 2.220   |       |
| $C_{32}H_{34}ClN_5Zn$                                    |   |       |
| Zinc(II) texaphyrin chloride                             | 2.225   |       |
| $C_{32}H_{34}Cl_4I_4N_2O_5$                              |   |       |
| Rose Bengal, bis(triethylammonium) salt                  |   |       |
| 1.180  |   |       |
| $C_{32}H_{34}N_4O_4$                                     | Deuteroporphyrin, dimethyl ester  | 2.198 |
| $C_{32}H_{34}N_6O_4Zn$                                   |   |       |
| Zinc(II) 5,10-dinitroetioporphyrin I                     | 2.96  |       |
| Zinc(II) 5,15-dinitroetioporphyrin I                     | 2.98  |       |
| $C_{32}H_{35}MnN_5O$                                     |   |       |
| Manganese(II) texaphyrin, hydroxide                      | 2.222   |       |
| $C_{32}H_{35}N_7O_6$                                     | 5,10,15-Trinitroetioporphyrin I   | 2.100 |
| $C_{32}H_{36}D_2N_4$                                     | Etioporphyrin- <i>d</i> <sub>2</sub>  | 2.61  |
|  | 5,10,15,20-Tetrapropylporphine- <i>d</i> <sub>2</sub>   | 2.66  |
| $C_{32}H_{36}N_4Zn$                                      | Zinc(II) etioporphyrin  | 2.94  |
| $C_{32}H_{36}N_6O_4$                                     | 5,10-Dinitroetioporphyrin I   | 2.95  |
|  | 5,15-Dinitroetioporphyrin I   | 2.97  |
| $C_{32}H_{37}N_5O_2$                                     | 5-Nitroetioporphyrin I  | 2.99  |
| $C_{32}H_{38}N_4$  | Etioporphyrin I   | 2.93  |
|  | 5,10,15,20-Tetrapropylporphine  | 2.147 |
|  | 2,7,12,17-Tetrapropylporphycene   | 2.212 |
| $C_{32}H_{39}N_5$  | 5-Aminoetioporphyrin I  | 2.48  |
| $C_{33}H_{25}Cl_4I_4NO_5$                                | Rose Bengal, benzyl ester, triethylammonium salt  | 1.176 |
| $C_{33}H_{32}ClN_3$                                      | Victoria Blue B   | 3.107 |
| $C_{33}H_{32}N_4O_5$                                     | Purpurin 18   | 2.151 |
| $C_{33}H_{41}BF_4N_2O$                                   |   |       |
|  | 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-(2,2-dimethoxyethyl)-1,3,5-heptatrienyl]-1,1,3-trimethylindolinium, tetrafluoroborate | 3.99  |
| $C_{34}H_{14}Cl_2O_2$                                    |   |       |
|  | 6,15-Dichloroisoviolanthrone  | 3.4   |
| $C_{34}H_{14}N_2O_6$                                     | 16,17-Dinitroviolanthrone   | 3.3   |
| $C_{34}H_{16}O_2$  | Anthra[9,1,2- <i>cde</i> ]benzo[ <i>rs</i> ]pentaphene-5,10-dione   | 3.1   |
| $C_{34}H_{22}N_2O_2Pt$                                   |   |       |
|  | 4,7-Diphenyl-1,10-phenanthroline(2,3-naphthalenediolato)platinum(II)  | 3.76  |
| $C_{34}H_{23}Cl_4I_4O_5S$                                |   |       |
|  | Rose Bengal, benzyl ester, diphenylmethylsulfonium salt   | 1.175 |
| $C_{34}H_{32}Cl_2N_4O_4Sn^{2+}$                          |   |       |
|  | Dichlorotin(IV) protoporphyrin  | 2.172 |
| $C_{34}H_{32}MgN_4O_4$                                   |   |       |
|  | Magnesium(II) protoporphyrin  | 2.170 |
| $C_{34}H_{32}N_4O_4Zn$                                   |   |       |
|  | Zinc(II) protoporphyrin IX  | 2.173 |
| $C_{34}H_{34}N_4O_4$                                     | Protoporphyrin IX   | 2.165 |
| $C_{34}H_{34}N_4O_6$                                     | 7,12-Diformyldeuteroporphyrin IX dimethyl ester   | 2.188 |
| $C_{34}H_{36}CoN_4O_6$                                   |   |       |
|  | Cobalt(III) hematoporphyrin   | 2.155 |
| $C_{34}H_{36}CuN_4O_6$                                   |   |       |
|  | Copper(II) hematoporphyrin IX   | 2.156 |

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| $C_{34}H_{36}MnN_4O_6$       | Manganese(III) hematoporphyrin  | 2.159 |
| $C_{34}H_{36}N_4NiO_6$       | Nickel(II) hematoporphyrin IX   | 2.160 |
| $C_{34}H_{36}N_4O_5$         | Monohydroxyethyl vinyl deuteroporphyrin   | 2.195 |
| $C_{34}H_{36}N_4O_6$         | Chlorin a <sub>6</sub>  | 2.200 |
| $C_{34}H_{36}N_4O_6Pd$       | Palladium(II) hematoporphyrin IX  | 2.161 |
| $C_{34}H_{36}N_4O_6Pt$       | Platinum(II) hematoporphyrin IX   | 2.162 |
| $C_{34}H_{38}N_4O_6$         | Hematoporphyrin IX  | 2.154 |
|                              | Isohematoporphyrin  | 2.163 |
| $C_{34}H_{40}EuN_5O_2$       | Europium(III) dimethyltexaphyrin dihydroxide  | 2.221 |
| $C_{34}H_{40}N_5O_2Sm$       | Samarium(II) dimethyltexaphyrin dihydroxide   | 2.223 |
| $C_{34}H_{42}B_2F_8N_3$      | 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-(1-piperidinio)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, bis(tetrafluoroborate) | 3.100 |
| $C_{35}H_{32}MgN_4O_5$       | Protochlorophyllide   | 2.20  |
| $C_{35}H_{36}N_4O_5$         | Pheophorbide <i>a</i>   | 2.22  |
|                              | 7(12)-Formyl-12(7)-vinyldeuteroporphyrin IX dimethyl ester  | 2.194 |
| $C_{35}H_{42}N_4O_6$         | Phycocyanobilin dimethyl ester  | 3.33  |
| $C_{36}H_{16}CuN_8O_8$       | Copper(II) tetracarboxyphthalocyanine   | 2.40  |
| $C_{36}H_{18}Br_2O_4$        | Dibromo-16,17-dimethoxyviolanthrone   | 3.2   |
| $C_{36}H_{20}EuF_9N_2O_6S_3$ | 1,10-Phenanthrolinebis(1-thienyl-4,4,4-trifluoro-1,3-butanedionato)europium(III)  | 3.140 |
| $C_{36}H_{20}N_4Zn$          | Tetrabenzoporphinatozinc(II)  | 2.214 |
| $C_{36}H_{23}BrN_6Ru^{2+}$   | 5-Bromo-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion  | 1.119 |
| $C_{36}H_{23}ClN_6Ru^{2+}$   | 5-Chloro-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion   | 1.123 |
| $C_{36}H_{24}IrN_6^{3+}$     | Tris(1,10-phenanthroline)iridium(III) ion   | 1.307 |
| $C_{36}H_{24}N_6Os^{2+}$     | Tris(1,10-phenanthroline)osmium(II) ion   | 1.308 |
| $C_{36}H_{24}N_6Ru^{2+}$     | Tris(1,10-phenanthroline)ruthenium(II) ion  | 1.309 |
| $C_{36}H_{36}D_2N_4O_4$      | Protoporphyrin IX- <i>d</i> <sub>2</sub> , dimethyl ester   | 2.167 |
| $C_{36}H_{36}MgN_4O_4$       | Magnesium(II) protoporphyrin, dimethyl ester  | 2.168 |
| $C_{36}H_{36}N_4O_3$         | Mesovordin methyl ester   | 2.227 |
| $C_{36}H_{36}N_4O_4Pd$       | Palladium(II) protoporphyrin dimethyl ester   | 2.171 |
| $C_{36}H_{36}N_4O_4Zn$       | Zinc(II) protoporphyrin, dimethyl ester   | 2.169 |
| $C_{36}H_{38}N_4O_4$         | Protoporphyrin IX, dimethyl ester   | 2.166 |
| $C_{36}H_{38}N_4O_6$         | Photoprotoporphyrin IX dimethyl ester   | 2.196 |
| $C_{36}H_{38}N_4O_8$         | Coproporphyrin I  | 2.204 |
|                              | Coproporphyrin III  | 2.205 |
| $C_{36}H_{40}CdN_4O_4$       | Cadmium(II) mesoporphyrin IX, dimethyl ester  | 2.179 |
| $C_{36}H_{40}CuN_4O_4$       | Copper(II) mesoporphyrin IX, dimethyl ester   | 2.180 |
| $C_{36}H_{40}D_2N_4O_4$      | Mesoporphyrin IX- <i>d</i> <sub>2</sub> , dimethyl ester  | 2.178 |
| $C_{36}H_{40}HgN_4O_4$       | Mercury(II) mesoporphyrin IX, dimethyl ester  | 2.182 |
| $C_{36}H_{40}MgN_4O_4$       | Magnesium(II) mesoporphyrin IX, dimethyl ester  | 2.181 |
| $C_{36}H_{40}N_4O_4Pd$       | Palladium(II) mesoporphyrin IX, dimethyl ester  | 2.183 |
| $C_{36}H_{40}N_4O_4Zn$       | Zinc(II) mesoporphyrin IX, dimethyl ester   | 2.185 |
| $C_{36}H_{40}N_4O_5V$        | Vanadium(IV) (oxo)mesoporphyrin IX, dimethyl ester  | 2.184 |
| $C_{36}H_{40}N_4O_6^{2-}$    | 2,4-Di( $\alpha$ -methoxyethyl)deuteroporphyrin dianion   | 2.164 |
| $C_{36}H_{42}N_4O_4$         | Mesoporphyrin IX, dimethyl ester  | 2.177 |
| $C_{36}H_{42}N_4O_6$         | Hematoporphyrin dimethyl ester  | 2.158 |
| $C_{36}H_{44}CdN_4$          | 2,3,7,8,12,13,17,18-Octaethylporphinatocadmium(II)  | 2.74  |

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| $C_{36}H_{44}Cl_2N_4Sn$   | $C_{38}H_{52}MnN_6.2CH_4O_3S$  |
| 2,3,7,8,12,13,17,18-<br>Octaethylporphinatotin(IV) dichloride<br>2.82   | Manganese(II) 1,3,5,8-tetramethyl-2,4-<br>diethyl-6,7-di(3-<br>dimethylaminopropyl)porphyrin,<br>dimethanesulfonate 2.51 |
| $C_{36}H_{44}CuN_4$ 2,3,7,8,12,13,17,18-<br>Octaethylporphinacopper(II) 2.75  | $C_{38}H_{52}N_6.2CH_4O_3S$  |
| $C_{36}H_{44}D_2N_4$ 21,23-Dideutero-2,3,7,8,12,13,17,18-<br>octaethylporphine 2.54   | 1,3,5,8-Tetramethyl-2,4-diethyl-6,7-di(3-<br>dimethylaminopropyl)porphyrin,<br>dimethanesulfonate 2.49                   |
| $C_{36}H_{44}InN_4$ Octaethylporphinatoindium(II) 2.77  | $C_{38}H_{52}N_6Zn.2CH_4O_3S$  |
| $C_{36}H_{44}N_4OTi$  | Zinc(II) 1,3,5,8-tetramethyl-2,4-diethyl-6,7-<br>di(3-dimethylaminopropyl)porphyrin,<br>dimethanesulfonate 2.52          |
| $C_{36}H_{44}N_4OV$   | $C_{39}H_{20}Cl_4I_5O_5$   |
| Octaethylporphinatooxovanadium(IV) 2.79   | Rose Bengal, benzyl ester, diphenyliodonium<br>salt 1.174  |
| $C_{36}H_{44}N_4Pb$ 2,3,7,8,12,13,17,18-<br>Octaethylporphinatolead(II) 2.76  | $C_{39}H_{34}Cl_3N_3O_4S_2$  |
| $C_{36}H_{44}N_4Pd$ 2,3,7,8,12,13,17,18-<br>Octaethylporphinatopalladium(II) 2.80   | IR 140 3.25  |
| $C_{36}H_{44}N_4Sc^+$   | $C_{40}H_{24}$ Mesodiphenylhelianthrene 1.139  |
| Octaethylporphinatoscandium(III) 2.81   | $C_{40}H_{38}N_4O_{16}$ Uroporphyrin I 2.203   |
| $C_{36}H_{44}N_4Zn$ 2,3,7,8,12,13,17,18-<br>Octaethylporphinatzinc(II) 2.83   | $C_{40}H_{40}Cl_4I_4O_{11}$  |
| $C_{36}H_{46}D_2N_4$ Octaethylchlorin- $d_2$ 2.55   | Rose Bengal complexed with dicyclohexyl-<br>18-crown-8 1.181   |
| $C_{36}H_{46}N_4$ 2,3,7,8,12,13,17,18-Octaethylporphine 2.73  | $C_{40}H_{46}N_4O_8$ Coproporphyrin III, tetramethyl ester 2.206   |
| $C_{36}H_{48}N_4$ Octaethylchlorin 2.84   | $C_{40}H_{46}N_6O_8S_2Zn$  |
| $C_{37}H_{39}N_4O_7$ Coproverdin II trimethyl ester 2.229   | Zinc(II) porphyrin c 2.153   |
| $C_{37}H_{42}N_4O_2$ Zinc(II) etiopurpurin ethyl ester 2.17   | $C_{40}H_{47}Cl_4I_4NO_5$  |
| $C_{37}H_{43}D_2N_4O$   | Rose Bengal, octyl ester, tributylammonium<br>salt 1.189   |
| 5-Formyloctaethylporphyrin- $d_2$ 2.149   | $C_{40}H_{48}N_6O_8S_2$  |
| $C_{37}H_{45}N_4O$ 5-Formyloctaethylporphyrin 2.150   | Porphyrin c 2.152  |
| $C_{37}H_{46}CuN_4$ 2,3,7,8,12,13,17,18-Octaethyl-5-<br>methylporphinatocopper(II) 2.86   | $C_{40}H_{52}N_5^{2+}$ 3,8,12,13,17,22-Hexaethyl-2,7,18,23-<br>tetramethylsapphyrin, diprotonated<br>2.213               |
| $C_{37}H_{46}D_2N_4$ <i>meso</i> -Methyloctaethylporphine- $d_2$ 2.56   | $C_{41}H_{50}N_4O_2$ 2,3,7,8,12,13,17,18-Octaethyl-5-<br>porphinepropenoic acid ethyl ester 2.201                        |
| <i>N</i> -Methyloctaethylporphyrin- $d_2$ 2.57  | $C_{41}H_{52}Cl_2N_4O_2Sn$   |
| $C_{37}H_{46}N_4Zn$ 2,3,7,8,12,13,17,18-Octaethyl-5-<br>methylporphinatzinc(II) 2.87  | Tin(IV) dichloro[octaethylidihydropurpurin<br>ethyl ester] 2.15  |
| $C_{37}H_{48}N_4$ <i>meso</i> -Methyloctaethylporphine 2.85   | $C_{41}H_{52}N_4O_2$ Octaethylpurpurin ethyl ester 2.16  |
| <i>N</i> -Methyloctaethylporphyrin 2.88   | $C_{41}H_{54}N_4O_2$ Octaethylidihydropurpurin ethyl ester 2.14  |
| $C_{38}H_{45}N_5O_5$ (Z)-Dimethyl 7-[2-(dimethylamino)-2-<br>oxoethyl]-8-ethylidene-7,8-dihydro-<br>3,7,12,17-tetramethylporphine-2,18-<br>dipropionate 2.190 | $C_{42}H_{23}N_3O_6$ 4,5'-Dibenzoylaminoanthrimide 3.75  |
| $C_{38}H_{46}N_4O_4$ Mesoporphyrin IX, diethyl ester 2.176  | $C_{42}H_{26}N_{10}Zn$   |
| $C_{38}H_{46}N_4O_8$ Hematoporphyrin diacetate 2.157  | Zinc(II) phthalocyaninebis(pyridine) 2.25  |
| $C_{38}H_{47}N_5O_5$ (Z)-Dimethyl 7-[2-(dimethylamino)-2-<br>oxoethyl]-8-ethyl-7,8-dihydro-3,7,12,17-<br>tetramethylporphine-2,18-dipropionate<br>2.189       | $C_{42}H_{28}$ Rubrene 1.278   |
| $C_{38}H_{52}CoN_6.2CH_4O_3S$   | $C_{42}H_{48}D_2N_4$ 2,3,7,8,12,13,17,18-Octaethyl-5-<br>phenylporphine- $d_2$ 2.58                                      |
| Cobalt(II) 1,3,5,8-tetramethyl-2,4-diethyl-<br>6,7-di(3-dimethylaminopropyl)porphyrin,<br>dimethanesulfonate 2.50   | $C_{42}H_{50}N_4$ 2,3,7,8,12,13,17,18-Octaethyl-5-<br>phenylporphine 2.89  |
|   | $C_{43}H_{58}N_4O_4$ Methyl acetal of oxidized octaethylpurpurin<br>ethyl ester 2.7                                      |

|                                       |  |       |                          |   |       |
|---------------------------------------|--|-------|--------------------------|---|-------|
| $C_{44}H_{16}Cl_8N_4O_{12}S_4Zn^{4-}$ | 5,10,15,20-Tetrakis(2,6-dichloro-3-sulfonatophenyl)porphinatozincate(II) ion | 2.107 | $C_{44}H_{28}AlClN_4$    | 5,10,15,20-Tetraphenylporphinato(chloro)aluminum(III) ion               | 2.138 |
| $C_{44}H_{24}Cl_2N_4O_{12}S_4Sn^{4-}$ | Dichloro[5,10,15,20-tetrakis(4-sulfonatophenyl)porphinato]stannate(IV) ion   | 2.131 | $C_{44}H_{28}CdN_4$      | 5,10,15,20-Tetraphenylporphinatocadmium(II)                             | 2.137 |
| $C_{44}H_{24}Cl_4D_2N_4$              | 5,10,15,20-Tetrakis(2-chlorophenyl)porphine- $d_2$                           | 2.62  | $C_{44}H_{28}Cl_2N_4Sn$  | Dichloro(5,10,15,20-tetraphenylporphinato)tin(IV)                       | 2.141 |
|                                       | 5,10,15,20-Tetrakis(3-chlorophenyl)porphine- $d_2$                           | 2.63  | $C_{44}H_{28}CoN_4$      | 5,10,15,20-Tetraphenylporphinatocobalt(II)                              | 2.139 |
|                                       | 5,10,15,20-Tetrakis(4-chlorophenyl)porphine- $d_2$                           | 2.64  | $C_{44}H_{28}CuN_4$      | 5,10,15,20-Tetraphenylporphinatocuppper(II)                             | 2.140 |
| $C_{44}H_{24}Cl_4I_6O_5$              | Rose Bengal, bis(diphenyliodonium) salt                                      | 1.179 | $C_{44}H_{28}D_2N_4$     | 5,10,15,20-Tetraphenylporphine- $d_2$                                   | 2.65  |
| $C_{44}H_{24}F_4N_4Zn$                | Zinc(II) tetrakis(2-fluorophenyl)porphyrin                                   | 2.109 | $C_{44}H_{28}FeN_4^+$    | Iron(III) 5,10,15,20-tetraphenylporphyrin                               | 2.143 |
| $C_{44}H_{24}N_4O_{12}PdS_4^{4-}$     | 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphinatopalladate(II) ion            | 2.130 | $C_{44}H_{28}GaN_4$      | 5,10,15,20-Tetraphenylporphinatogallium(II)                             | 2.142 |
| $C_{44}H_{24}N_4O_{12}S_4Yb^{4-}$     | 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphinatoytterbium(II)                | 2.132 | $C_{44}H_{28}MnN_4^+$    | Manganese(III) 5,10,15,20-tetraphenylporphyrin                          | 2.144 |
| $C_{44}H_{24}N_4O_{12}S_4Zn^{4-}$     | 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphinatozincate(II) ion              | 2.133 | $C_{44}H_{28}N_4Zn$      | 5,10,15,20-Tetraphenylporphinatozinc(II)                                | 2.146 |
| $C_{44}H_{26}$                        | Mesodiphenylbenzheianthrene  | 1.303 | $C_{44}H_{28}NiN_4$      | 5,10,15,20-Tetraphenylporphinatonickel(II)                              | 2.145 |
| $C_{44}H_{26}Br_4N_4$                 | 5,10,15,20-Tetrakis(4-bromophenyl)porphine                                   | 2.102 | $C_{44}H_{30}D_2N_4$     | Tetraphenylchlorin- $d_2$   | 2.53  |
| $C_{44}H_{26}Cl_4N_4$                 | 5,10,15,20-Tetrakis(2-chlorophenyl)porphine                                  | 2.104 | $C_{44}H_{30}N_4$        | 5,10,15,20-Tetraphenylporphine  | 2.136 |
|                                       | 5,10,15,20-Tetrakis(3-chlorophenyl)porphine                                  | 2.105 | $C_{44}H_{30}N_4O_4$     | 5,10,15,20-Tetrakis(2-hydroxyphenyl)porphine                            | 2.111 |
|                                       | 5,10,15,20-Tetrakis(4-chlorophenyl)porphine                                  | 2.106 |                          | 5,10,15,20-Tetrakis(3-hydroxyphenyl)porphine                            | 2.112 |
| $C_{44}H_{26}F_4N_4$                  | 5,10,15,20-Tetrakis(2-fluorophenyl)porphine                                  | 2.108 |                          | 5,10,15,20-Tetrakis(4-hydroxyphenyl)porphine                            | 2.113 |
|                                       | 5,10,15,20-Tetrakis(4-fluorophenyl)porphine                                  | 2.110 | $C_{44}H_{32}N_4$        | Tetraphenylchlorin  | 2.67  |
| $C_{44}H_{26}I_4N_4$                  | 5,10,15,20-Tetrakis(4-iodophenyl)porphine                                    | 2.114 | $C_{44}H_{34}N_4$        | <i>trans</i> -Tetraphenylbacteriochlorin                                | 2.101 |
| $C_{44}H_{26}N_4O_{12}S_4^{4-}$       | 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphine                               | 2.129 | $C_{44}H_{36}CdN_8^{4+}$ | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatocadmium(II) ion   | 2.118 |
|                                       |  |       | $C_{44}H_{36}CoN_8^{5+}$ | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatocobalt(III) ion   | 2.119 |
|                                       |  |       | $C_{44}H_{36}CuN_8^{4+}$ | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatocuppper(II) ion   | 2.120 |
|                                       |  |       | $C_{44}H_{36}FeN_8^{4+}$ | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatoiron(II) ion      | 2.121 |
|                                       |  |       | $C_{44}H_{36}LuN_8^{5+}$ | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatolutetium(III) ion | 2.122 |

|                           |   |       |
|---------------------------|---|-------|
| $C_{44}H_{36}MgN_8^{4+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatomagnesium(II) ion   | 2.123 |
| $C_{44}H_{36}MnN_8^{5+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatomanganese(III) ion  | 2.124 |
| $C_{44}H_{36}N_8Ni^{4+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatonickel(II) ion  | 2.125 |
| $C_{44}H_{36}N_8Pd^{4+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatopalladium(II) ion   | 2.126 |
| $C_{44}H_{36}N_8Sn^{6+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatotin(IV) ion   | 2.127 |
| $C_{44}H_{36}N_8Zn^{4+}$  | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphinatozinc(II) ion  | 2.128 |
| $C_{44}H_{38}N_8^{4+}$    | 5,10,15,20-Tetrakis(1-methylpyridinium-2-yl)porphine  | 2.115 |
|                           | 5,10,15,20-Tetrakis(1-methylpyridinium-3-yl)porphine  | 2.116 |
|                           | 5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphine  | 2.117 |
| $C_{44}H_{48}BF_4N_3$     | 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-[3-(1,3,3-trimethyl-2-indolylidene)-2-propenyl]-1,3,5-heptatrienyl]- 1,1,3-trimethylindolium, tetrafluoroborate | 3.101 |
| $C_{44}H_{54}N_4O_8$      | [22]Coproporphyrin II   | 2.6   |
| $C_{44}H_{57}N_5O_5Sn$    | (Z)-2,18-Di(methoxycarbonylethyl)-7- [2-(dimethylamino)-2-oxoethyl]- 8-heptyl-7,8-dihydro- 3,7,12,17-tetramethylporphinatotin(IV)                             | 2.192 |
| $C_{44}H_{57}N_5O_5Zn$    | (Z)-2,18-Di(methoxycarbonylethyl)- 7-[2-(dimethylamino)- 2-oxoethyl]- 8-heptyl-7,8-dihydro- 3,7,12,17-tetramethylporphinatozinc(II)                           | 2.193 |
| $C_{44}H_{59}N_5O_5$      | (Z)-Dimethyl 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro- 3,7,12,17-tetramethylporphine- 2,18-dipropionate  | 2.191 |
| $C_{46}H_{36}FeN_8O_4$    | Iron(III) bis[2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate]  | 3.89  |
| $C_{46}H_{36}N_8NiO_4$    | Nickel(II) bis[2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate]   | 3.90  |
| $C_{47}H_{32}Cl_4I_4O_6$  | Rose Bengal, benzyl ester, 2,4,6-triphenylpyrylium salt   | 1.177 |
| $C_{48}H_{26}N_4O_8^{4-}$ | 5,10,15,20-Tetrakis(4-carboxyphenyl)porphine  | 2.103 |
| $C_{48}H_{28}CdN_4$       | Cadmium(II) diphenyltetraporphyrin  | 2.215 |
| $C_{48}H_{28}MgN_4$       | Magnesium(II) diphenyltetraporphyrin  | 2.216 |
| $C_{48}H_{28}N_4Zn$       | Zinc(II) diphenyltetraporphyrin   | 2.217 |
| $C_{48}H_{30}N_6O_6OsS_2$ | Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthrolineosmium(II)  | 1.117 |
| $C_{48}H_{30}N_6O_6RuS_2$ | Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthroline ruthenium(II)  | 1.118 |
| $C_{48}H_{32}N_6O_6^{2+}$ | (4,7-Diphenyl-1,10-phenanthroline)bis(1,10-phenanthroline)osmium(II) ion  | 1.141 |
| $C_{48}H_{48}AlClN_8$     | Chloro-2,9,16,23-[tetrakis(1,1-dimethylethyl)phthalocyaninato]aluminate(III)  | 2.42  |
| $C_{48}H_{48}CuN_8$       | Copper(II) 2,9,16,23-tetra- <i>tert</i> -butylphthalocyanine  | 2.43  |
| $C_{48}H_{48}MgN_8$       | 2,9,16,23-[Tetrakis(1,1-dimethylethyl)phthalocyaninato]magnesium(II)  | 2.44  |
| $C_{48}H_{50}N_8$         | 2,9,16,23-Tetra- <i>tert</i> -butylphthalocyanine   | 2.41  |
| $C_{48}H_{66}N_4^{2+}$    | [26] Porphyrin  | 2.210 |
| $C_{51}H_{67}CoN_6O_{12}$ | Hexamethyl Co $\alpha$ Co $\beta$ -dicyano-7-de(carboxymethyl)-7,8-didehydrocobyrinate  | 3.55  |
| $C_{52}H_{32}Cl_4I_4O_5P$ | Rose Bengal, benzyl ester, benzyltriphenylphosphonium salt  | 1.173 |
| $C_{52}H_{44}D_2N_4$      | Octamethyltetraphenylporphyrin- <i>d</i> <sub>2</sub>   | 2.59  |
| $C_{52}H_{46}N_4$         | Octamethyltetraphenylporphyrin  | 2.90  |
| $C_{54}H_{32}N_4Zn$       | Zinc(II) triphenyltetraporphyrin  | 2.218 |
| $C_{55}H_{53}N_6O_7$      | Mesoporphyrin [4-(diphenylmethyleaminocarbonyl-2-nitrophenylmethyl) monoester   | 2.187 |
| $C_{55}H_{70}MgN_4O_5$    | Protochlorophyll  | 2.23  |
| $C_{55}H_{70}MgN_4O_6$    | Chlorophyll <i>b</i>  | 2.4   |
| $C_{55}H_{72}MgN_4O_5$    | Chlorophyll <i>a</i>  | 2.3   |

|                               |   |       |                              |   |
|-------------------------------|---|-------|------------------------------|---|
| $C_{55}H_{72}MgN_4O_6$        | Bacteriochlorophyll <i>b</i>  | 2.2   | $C_{74}H_{90}N_8Zn_2$        | Porphine, ethanediylbis[5,5'-<br>(2,3,7,8,12,13,17,18-octaethyl-,<br>biszinc(II) 2.71 |
| $C_{55}H_{72}N_4O_5$          | Protopheophytin   | 2.21  | $C_{74}H_{92}CuN_8$          | Porphine, ethanediylbis[5,5'-<br>(2,3,7,8,12,13,17,18-octaethyl-,<br>copper(II) 2.69  |
| $C_{55}H_{72}N_4O_6$          | Pheophytin <i>b</i>   | 2.13  | $C_{74}H_{94}N_8$            | Ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethylporphine)] 2.68                      |
| $C_{55}H_{74}MgN_4O_6$        | Bacteriochlorophyll <i>a</i>  | 2.1   | $C_{76}H_{70}N_8O_{10}$      | Mesoporphyrin di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) ester 2.174      |
| $C_{55}H_{74}N_4O_5$          | Pheophytin <i>a</i>   | 2.12  | $C_{76}H_{72}N_6O_6$         | Mesoporphyrin di[4-(diphenylmethylaminocarbonylphenylmethyl) ester 2.175              |
| $C_{55}H_{74}N_4O_6$          | Bacteriopheophytin <i>b</i>   | 2.19  | $C_{77}H_{88}N_8O_{12}$      | 1,11-Undecanediylbis[3,8,12,17-tetramethyl-2,7,18-tris(2-carboxyethyl)porphine 2.209  |
| $C_{55}H_{76}N_4O_6$          | Bacteriopheophytin <i>a</i>   | 2.18  | $C_{82}H_{106}Cu_2N_8$       | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octapropyl-, bis copper(II) 2.72    |
| $C_{56}H_{55}N_6O_7$          | Mesoporphyrin [4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) methyl ester               | 2.186 | $C_{84}H_{102}N_8O_2Si_3$    | Bis(tri- <i>n</i> -hexyloxysiloxo)-2,3-naphthalocyaninatosilicon 2.11                 |
| $C_{56}H_{62}N_8^{4+}$        | 5,10,15,20-Tetrakis(4-trimethylammoniophenyl)porphine   | 2.134 | $C_{92}H_{85}N_{15}O_3^{6+}$ | Bis-porphyrin 2.148   |
| $C_{56}H_{68}Cl_4CuN_{16}S_4$ | Alcian Blue   | 2.45  |                              |   |
| $C_{60}$                      | Carbon sixty-atom molecule  | 1.120 |                              |   |
| $C_{60}H_{48}ClN_7O$          | <i>N</i> -[4-[(7-Chloro-4-quinolyl)amino]butyl]-5,10,15,20-tetraphenylporphine-2-propionamide | 2.202 |                              |   |
| $C_{64}H_{56}AlClN_8$         | Aluminum(III) chloro[2,11,20,29-tetra- <i>tert</i> -butylnaphthalocyanine]                    | 2.9   |                              |   |
| $C_{64}H_{56}CuN_8$           | Copper(II) 2,11,20,29-tetra- <i>tert</i> -butylnaphthalocyanine                               | 2.10  |                              |   |
| $C_{64}H_{58}N_8$             | 2,11,20,29-Tetra- <i>tert</i> -butylnaphthalocyanine  | 2.8   |                              |   |
| $C_{64}H_{80}N_8O_8Zn$        | Zinc(II) 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine  | 2.26  |                              |   |
| $C_{69}H_{72}N_8O_{12}$       | 1,3-Propanediylbis[3,8,12,17-tetramethyl-2,7,18-tris(2-carboxyethyl)porphine                  | 2.208 |                              |   |
| $C_{70}$                      | Carbon seventy-atom molecule  | 1.121 |                              |   |
| $C_{70}H_{47}Cl_4I_4O_5P_2$   | Rose Bengal,<br>bis(benzyltriphenylphosphonium) salt  | 1.178 |                              |   |
| $C_{72}H_{78}N_8O_{12}$       | 1,6-Hexanediylbis[3,8,12,17-tetramethyl-2,7,18-tris(2-carboxyethyl)porphine                   | 2.207 |                              |   |
| $C_{74}H_{90}CuN_8Zn$         | Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, copper(II)zinc(II) 2.70         |       |                              |   |

## 11. Chemical Name Index

- Acetamide, *N*-[4-[[4-(diethylamino)-2-methylphenyl]imino]-4,5-dihydro-5-oxo-1-(4-bromophenyl)pyrazol-3-yl]- 3.150
- Acetamide, *N*-[4-[[4-(diethylamino)-2-methylphenyl]imino]-4,5-dihydro-5-oxo-1-(4-chlorophenyl)pyrazol-3-yl]- 3.151
- Acetamide, *N*-[4-[[4-(diethylamino)-2-methylphenyl]imino]-4,5-dihydro-5-oxo-1-(3-methoxyphenyl)pyrazol-3-yl]- 3.152
- Acetamide, *N*-[4-[[4-(diethylamino)-2-methylphenyl]imino]-4,5-dihydro-5-oxo-1-(3-methylphenyl)pyrazol-3-yl]- 3.153
- Acetamide, *N*-[4-[[4-(diethylamino)-2-methylphenyl]imino]-4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)pyrazol-3-yl]- 3.155
- Acetamide, *N*-[4-[(2-hydroxy-5-methylphenyl)azo]phenyl]- 3.56
- 3-Acetoallopssoralen 1.193
- 3-Acetoanglicin 1.197
- 5'-Aceto-4,8-dimethylpsoralen 1.210
- 3-Acetoisopseudopsoralen 1.209
- 5'-Aceto-8-methylpsoralen 1.211
- 2'-Acetonaphthone 1.1
- Acetophenone 1.2
- Acetophenone, 4'-cyano- 1.3
- Acetophenone, 3'-methoxy- 1.4
- Acetophenone, 4'-methoxy- 1.5
- Acetophenone, 2-methyl-, biradical 1.6
- 3-Acetopseudoisopsonralen 1.212
- (*E*)-6-(Acetylamino)-2'-bromo-6'-cyano-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-3-methoxyazobenzene 3.57
- (*E*)-6-(Acetylamino)-2'-bromo-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-3-methoxy-6'-nitroazobenzene 3.58
- (*E*)-6-(Acetylamino)-2'-chloro-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-3-methoxy-6'-nitroazobenzene 3.59
- (*E*)-6-(Acetylamino)-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-3-methoxy-6'-nitroazobenzene 3.60
- p*-Acetylbenzonitrile 1.3
- 2-Acetyl naphthalene 1.1
- 9-Acetoxy-11,12-dibenzoyl-9,10-dihydro-9,10-ethenoanthracene 1.143
- [9-(Acetoxy)-9,10-dihydro-9,10-ethenoanthracene-11,12-diyl]bis[phenylmethanone 1.143
- 2-Acetylphenothiazine 1.241
- 6-*O*-Acetyl Rose Bengal ethyl ester 1.170
- Acid Pure Sky Blue 3.7
- Acid Pure Sky Blue Anthraquinone 3.7
- Acridine 1.7
- Acridine, 3,6-diamino- 1.9
- 9-Acridinethione, 10-methyl- 1.8
- Acridinium, 3,6-diamino-10-methyl- 1.10
- Acriflavine cation 1.10
- Active Brilliant Sky Blue 2KT 3.8
- Active Yellow 2KT 3.9
- Adriamycin 3.111
- Afloqualone 3.163
- Alcian Blue 2.45
- Alizarin 1.61
- Allopsoralen 1.11
- Aluminum(III), chloro[2,11,20,29-tetrakis(1,1-dimethylethyl)tetranaphtho[2,3-*b*:2',3'-*g*:2'',3''-1:2'',3'''-*q*]porphyrazine 2.9
- Aluminum, chloro(trisulfophthalocyaninato)- 2.28
- Aluminum(III) chloro[2,11,20,29-tetra-*tert*-butylnaphthalocyanine] 2.9
- Aluminum(III) chloro-2,9,16,23-[tetrakis(1,1-dimethylethyl)phthalocyanine] 2.42
- Aluminum(III) chloro(5,10,15,20-tetraphenylporphyrin) 2.138
- Aluminum(III) 1-(2-hydroxyphenylazo)-2-naphtholate 3.122
- Aluminum(III) sulfophthalocyanine 2.30
- Ambramycin 3.108
- 1-Aminoanthraquinone 1.40
- 2-Aminoanthraquinone 1.41
- 5-Amino-6-bromo-9-diethylaminobenzo[*a*]phenoxyazinium 3.15
- 1-(4-Aminocarbonylphenylazo)-3-(2-methoxyphenylaminocarbonyl)-2-naphthol 3.114
- 5-Amino-6,8-dibromo-9-ethylaminobenzo[*a*]phenoxyazinium 3.16
- 5-Amino-9-diethylaminobenzo[*a*]phenothiazinium 3.12
- 5-Amino-9-diethylaminobenzo[*a*]phenoxyazinium 3.17
- 5-Amino-9-diethylamino-2,6-diiodobenzo[*a*]phenoxyazinium 3.18
- 5-Amino-9-diethylamino-6-iodobenzo[*a*]phenothiazinium 3.13
- 5-Amino-9-diethylamino-2-iodobenzo[*a*]phenoxyazinium 3.20
- 5-Amino-9-diethylamino-6-iodobenzo[*a*]phenoxyazinium 3.21
- 5-Amino-9-ethylamino-6,8-diiodobenzo[*a*]phenoxyazinium 3.19
- 5-Aminoetioporphyrin I 2.48
- α-Amino-2-(formylamino)-γ-oxobenzenebutanoic acid 1.76
- 1-Amino-2-hydroxyanthraquinone 1.42
- 1-Amino-4-hydroxyanthraquinone 1.43
- 1-Amino-4-hydroxy-2-phenoxyanthraquinone 1.44
- 1-Amino-4-hydroxy-2-[4-(phenylaminosulfonyl)phenoxy]anthraquinone 1.45

|   |       |
|---|-------|
| 1-Amino-2-methylanthraquinone   | 1.46  |
| 4-(Aminomethylene)-3-methyl-1-phenyl-2-pyrazoline-5-selone  | 3.148 |
| 4-(Aminomethylene)-3-methyl-1-phenyl-2-pyrazoline-5-thione  | 3.149 |
| 6-Aminophenalenone  | 1.236 |
| Angelicin   | 1.12  |
| Angelicin, 4-methyl-  | 1.203 |
| Anthanthrene  | 1.138 |
| Anthra[9,1,2-cde]benzo[rst]pentaphene-5,10-dione  | 3.1   |
| Anthra[9,1,2-cde]benzo[rst]pentaphene-5,10-dione, dibromo-16,17-dimethoxy-  | 3.2   |
| Anthra[9,1,2-cde]benzo[rst]pentaphene-5,10-dione, 16,17-dinitro-  | 3.3   |
| Anthra[9,1,2-cde]benzo[rst]pentaphene-10,18-dione, 6,15-dichloro-   | 3.4   |
| Anthra[2,1-d:6,5-d']bisthiazole-6,12-dione, 1,8-diphenyl-   | 3.5   |
| Anthracene  | 1.13  |
| Anthracene, 9- <i>tert</i> -butyl-  | 1.24  |
| Anthracene, 1-chloro-   | 1.14  |
| Anthracene, 9-chloro-   | 1.15  |
| Anthracene, 9-cyano-  | 1.16  |
| Anthracene, 9,10-dibromo-   | 1.17  |
| Anthracene, 9,10-dichloro-  | 1.18  |
| Anthracene, 9,10-dicyano-   | 1.19  |
| Anthracene, 1,4-dimethoxy-9,10-diphenyl-  | 1.20  |
| Anthracene, 9,10-dimethyl-  | 1.21  |
| Anthracene, 2-(3,3-dimethyl-1-butenyl)-, ( <i>E</i> )-  | 1.22  |
| Anthracene, 2-(3,3-dimethyl-1-butenyl)-, ( <i>Z</i> )-  | 1.23  |
| Anthracene, 9,10-diphenyl-  | 1.25  |
| Anthracene, 9-methyl-   | 1.26  |
| Anthracene, 2-[2-(2-naphthyl)ethenyl]-, ( <i>E</i> )-   | 1.27  |
| Anthracene, 2-[2-(2-naphthyl)ethenyl]-, ( <i>Z</i> )-   | 1.28  |
| Anthracene, 9-phenyl-   | 1.29  |
| Anthracene, 2-(2-phenylethenyl)-, ( <i>Z</i> )-   | 1.30  |
| Anthracene, 2-(1-propenyl)-, ( <i>E</i> )-  | 1.32  |
| Anthracene, 2-( $\beta$ -styryl)-, ( <i>E</i> )-  | 1.31  |
| Anthracene, 2,6,9,10-tetracyano-  | 1.33  |
| Anthracene, 2-vinyl-  | 1.34  |
| 9-Anthracenecarbonitrile  | 1.16  |
| 1-Anthracenesulfonate ion   | 1.35  |
| 2-Anthracenesulfonate ion   | 1.36  |
| 2-Anthracenesulfonic acid, 1-amino-9,10-dihydro-9,10-dioxo-4-[3-[(2-sulfoxyethyl)sulfonyl]phenyl]amino]-, disodium salt               | 3.6   |
| Anthra[1,9-bc:4,10-b'c']dichromene  | 1.37  |
| Anthra[2,1,0-def:6,5,10-d'e'f']diisoquinoline, <i>N,N'</i> -dimethyl-   | 1.38  |
| Anthralin   | 1.68  |
| Anthralin conjugate base  | 1.69  |
| 9,10-Anthraquinone  | 1.39  |
| 9,10-Anthraquinone, 1-amino-  | 1.40  |
| 9,10-Anthraquinone, 2-amino-  | 1.41  |
| 9,10-Anthraquinone, 1-amino-2-hydroxy-  | 1.42  |
| 9,10-Anthraquinone, 1-amino-4-hydroxy-  | 1.43  |
| 9,10-Anthraquinone, 1-amino-4-hydroxy-2-phenoxy-  | 1.44  |
| 9,10-Anthraquinone, 1-amino-4-hydroxy-2-[4-(phenylaminosulfonyl)phenoxy]-   | 1.45  |
| 9,10-Anthraquinone, 1-amino-2-methyl-   | 1.46  |
| 9,10-Anthraquinone, 1-chloro-   | 1.47  |
| 9,10-Anthraquinone, 2-chloro-   | 1.48  |
| 9,10-Anthraquinone, 1,2-diamino-  | 1.49  |
| 9,10-Anthraquinone, 1,4-diamino-  | 1.50  |
| 9,10-Anthraquinone, 1,5-diamino-  | 1.51  |
| 9,10-Anthraquinone, 1,8-diamino-  | 1.52  |
| 9,10-Anthraquinone, 2,6-diamino-  | 1.53  |
| 9,10-Anthraquinone, 1,5-diamino-2-bromo-4,8-dihydroxy-  | 1.54  |
| 9,10-Anthraquinone, 1,5-diamino-4,8-dihydroxy-  | 1.55  |
| 9,10-Anthraquinone, 1,8-diamino-4,5-dihydroxy-  | 1.56  |
| 9,10-Anthraquinone, 2,5-diamino-1,8-dihydroxy-  | 1.57  |
| 9,10-Anthraquinone, 2,7-diamino-1,8-dihydroxy-  | 1.58  |
| 9,10-Anthraquinone, 1,4-diamino-2-methoxy-  | 1.59  |
| 9,10-Anthraquinone, 1,4-diamino-2-[4-(phenylaminosulfonyl)phenoxy]-   | 1.60  |
| 9,10-Anthraquinone, 1,2-dihydroxy-  | 1.61  |
| 9,10-Anthraquinone, 1,8-dihydroxy-  | 1.62  |
| 9,10-Anthraquinone, 1-hydroxy-  | 1.63  |
| 9,10-Anthraquinone, 2-hydroxy-  | 1.64  |
| 9,10-Anthraquinone, 1,4,5,8-tetraamino-   | 1.65  |
| 9,10-Anthraquinone, 1,4,5,8-tetrahydroxy-   | 1.66  |
| Anthrone  | 1.67  |
| Anthrone, 1,8-dihydroxy-  | 1.68  |
| Anthrone, 1,8-dihydroxy-, conjugate base  | 1.69  |
| ( <i>E</i> )-1-(2-Anthryl)-2-(2-naphthyl)ethylene   | 1.27  |
| ( <i>E</i> )-1-(2-Anthryl)-2-phenylethylene   | 1.31  |
| Azobenzene, 4-acetylamino-5-hydroxy-2-methyl-   | 3.56  |
| Azulene   | 1.70  |
| Bacteriochlorin, tetraphenyl- ( <i>trans</i> )  | 2.101 |
| Bacteriochlorophyll <i>a</i>  | 2.1   |
| Bacteriochlorophyll <i>b</i>  | 2.2   |
| Bacteriopheophytin <i>a</i>   | 2.18  |
| Bacteriopheophytin <i>b</i>   | 2.19  |
| Basic Blue 26   | 3.107 |
| Benoxaprofen  | 3.31  |
| Benzaldehyde  | 1.71  |
| Benzamide, 4-[3-(2-methoxyphenylaminocarbonyl)-2-hydroxy-1-naphthyl]-   | 3.114 |
| Benzamide, <i>N,N'</i> -(10,15,16,17-tetrahydro-5,10,15,17-tetraoxodinaphtho[2,3: <i>a</i> :2',3'- <i>i</i> ])carbazole-4,9-diyl)bis- | 3.75  |
| 1,2-Benzanthracene  | 1.72  |

- 2,3-Benzanthracene 1.291  
 Benz[*a*]anthracene 1.72  
 Benz[*a*]anthracene, 9,10-dimethyl- 1.73  
 Benz[*b*]anthracene 1.291  
 Benzene, 5-chloro-1,3-dimethoxy- 1.74  
 Benzene, 1,3-dihydroxy- 1.79  
 Benzene, 1,4-dihydroxy- 1.81  
 Benzene, 1,3,5-triphenyl- 1.75  
 Benzenebutanoic acid,  $\alpha$ -amino-2-(formylamino)- $\gamma$ -oxo- 1.76  
 Benzenebutanoic acid,  $\alpha$ ,2-diamino-3-hydroxy- $\gamma$ -oxo- 1.77  
 Benzenebutanoic acid,  $\alpha$ ,2-diamino- $\gamma$ -oxo- 1.78  
 1,3-Benzenediol, 4-chloro- 1.80  
 1,3-Benzenedisulfonamide, *N*-[5-hydroxy-8-[[2-(methylsulfonyl)-4-nitrophenyl]azo]-1-naphthalenyl-, conjugate base 3.120  
 Benzenesulfonamide, 4-[(1-amino-9,10-dihydro-4-hydroxy-9,10-dioxo-2-anthracyl)oxy]-*N*-phenyl- 1.45  
 Benzenesulfonamide, 4-[(1,4-diamino-9,10-dihydro-9,10-dioxo-2-anthracyl)oxy]-*N*-phenyl- 1.60  
 Benzenesulfonic acid, 2-[(4-amino-3-bromo-9,10-dihydro-9,10-dioxo-1-anthracyl)amino]-5-methyl-, monosodium salt 3.7  
 Benzenesulfonic acid, 4-[(4-amino-9,10-dihydro-9,10-dioxo-1-anthracyl)amino]phenyl]amino]-6-(2-chloro-1,3,5-triazin-4-yl)amino 3.8  
 Benzenesulfonic acid, 4-[(2-methoxy-5-(2-sulfatoethyl)sulfonylphenyl)azo-3-[2-hydroxy-5-methyl-imidaz-1-yl]-, disodium salt 3.9  
 Benzil 1.83  
 Benzil, 4,4'-dichloro- 1.84  
 Benzil, 4,4'-dimethoxy- 1.85  
 Benzil, 2,2',4,4',6,6'-hexamethyl- 1.86  
 Benzimidazo[2,10*a*]benz[*de*]isoquinolin-7-one, 4-benzoyl- 3.10  
 Benz[*a*]indeno[1,2,3-*hi*]aceanthrylene 1.277  
 Benzo[1,2,3-*kl*:4,5,6-*k'l*]dixanthene 1.87  
 Benzoic acid, 2-[6-(acetoxy)-2,4,5,7-tetraiodo-3-oxo-xanthen-9-yl]-3,4,5,6-tetrachloro-, ethyl ester 1.170  
 Benzoic acid, 2-(2,4,5,7-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-, methyl ester 1.164  
 Benzoic acid, 2-(2,4,5,7-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-, methyl ester, conjugate base 1.165  
 Benzoic acid, 2-(2,4,5,7-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-, [4-(1-methylethyl)phenyl]methyl ester, conjugate base 1.163  
 Benzoic acid, 2-(2,4,5,7-tetrabromo-6-hydroxy-3-oxoxanthen-9-yl)-, phenylmethyl ester, conjugate base 1.162  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, ethyl ester 1.182  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, ethyl ester, compound with triethylamine 1.183  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, methyl ester 1.187  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, methyl ester, conjugate base 1.188  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, [4-(1-methylethyl)phenyl]methyl ester 1.184  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, [4-(1-methylethyl)phenyl]methyl ester, conjugate base 1.185  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, octyl ester, compound with tributylamine 1.189  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester 1.171  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, benzyltriphenylphosphonium salt 1.173  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, compound with triethylamine 1.176  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, conjugate base 1.172  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, diphenyliodonium salt 1.174  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, diphenylmethylsulfonium salt 1.175  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-hydroxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, phenylmethyl ester, 2,4,6-triphenylpyrylium salt 1.177  
 Benzoic acid, 2,3,4,5-tetrachloro-6-(6-methoxy-2,4,5,7-tetraiodo-3-oxoxanthen-9-yl)-, methyl ester 1.186  
 Benzo[*d*]naphtho[1,2-*b*]pyran-6-one, 4-(6-deoxy- $\alpha$ -galactofuranosyl)-1-hydroxy-10,12-dimethoxy-8-methyl- 3.11  
 Benzophenone 1.88  
 Benzophenone, 4,4'-bis(dimethylamino)- 1.89  
 Benzophenone, 4,4'-dimethoxy- 1.90  
 Benzophenone, 4-fluoro- 1.91  
 Benzophenone, 4-(trifluoromethyl)- 1.92  
 Benzo[*a*]phenothiazine 1.93  
 Benzo[*b*]phenothiazine 1.94  
 Benzo[*c*]phenothiazine 1.95  
 Benzo[*a*]phenothiazinium, 5-amino-9-diethylamino- 3.12  
 Benzo[*a*]phenothiazinium, 5-amino-9-diethylamino-6-iodo- 3.13

- Benzo[*a*]phenothiazinium, 5-benzylamino-9-diethylamino- 3.14
- Benzo[*a*]phenoxazinium, 5-amino-6-bromo-9-diethylamino- 3.15
- Benzo[*a*]phenoxazinium, 5-amino-6,8-dibromo-9-diethylamino- 3.16
- Benzo[*a*]phenoxazinium, 5-amino-9-diethylamino- 3.17
- Benzo[*a*]phenoxazinium, 5-amino-9-diethylamino-2,6-diido- 3.18
- Benzo[*a*]phenoxazinium, 5-amino-9-diethylamino-2-iodo- 3.20
- Benzo[*a*]phenoxazinium, 5-amino-9-diethylamino-6-iodo- 3.21
- Benzo[*a*]phenoxazinium, 5-amino-9-ethylamino-6,8-diido- 3.19
- Benzo[*a*]phenoxazinium, 5-benzylamino-9-diethylamino- 3.22
- 1-Benzopyran-4-one, 2,3-diphenyl- 1.96
- 1-Benzopyran-4-one, 3-hydroxy-2-phenyl- 1.97
- 1-Benzopyran-4-one, 2-phenyl- 1.98
- [1]Benzopyrano[6,7,8-*ij*]quinolizin-11-one, 2,3,6,7-tetrahydro-9-methyl- 1.99
- 1,2-Benzopyrone 1.128
- 1,4-Benzoquinone, 2,6-diphenyl- 1.100
- 1,4-Benzoquinone, 2,6-diphenyl-, complex with Triphenylamine 1.101
- 1,4-Benzoquinone, tetrachloro- 1.102
- 1,4-Benzoquinone, tetrachloro-, complex with Anisole 1.103
- 1,4-Benzoquinone, tetrachloro-, complex with Durene 1.104
- 1,4-Benzoquinone, tetrachloro-, complex with Hexamethylbenzene 1.105
- 1,4-Benzoquinone, tetrachloro-, complex with 1,2,3-Trimethoxybenzene 1.106
- 1,4-Benzoquinone, tetramethyl- 1.107
- 1,2-Benzothiazine-3-carboxamide, 4-hydroxy-2-methyl-*N*-(2-pyridyl)- 1,1-dioxide 3.23
- 1,2-Benzothiazin-4-one, 2,3-dihydro-2-methyl-, 1,1-dioxide 3.24
- Benzothiazolium, 5-chloro-2-[2-[3-[(5-chloro-3-ethyl-2-benzothiazolidene)ethylidene]-2-(diphenylamino)-1-cyclopenten-1-yl)ethenyl]-3-ethyl-, perchlorate 3.25
- Benzothiazolium, 6-chloro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate 3.26
- Benzothiazolium, 3,6-dimethyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate 3.27
- Benzothiazolium, 3-ethyl-2-[7-(3-ethyl-2-benzothiazolidene)-1,3,5-heptatrienyl]-, iodide 3.194
- Benzothiazolium, 6-fluoro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate 3.28
- Benzothiazolium, 6-methoxy-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)-, tetrafluoroborate 3.29
- Benzothiazolium, 3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1,3,5-heptatrienyl]-, iodide 3.30
- 5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)- $\alpha$ -methyl- 3.31
- 3-Benzoxazolepropanesulfonic acid, 2-[4-(1,3-dibutyltetrahydro-4,6-dioxo-2-thioxo-5-pyrimidinylidene)-2-butenylidene]-, sodium salt 3.32
- Benzoxazolium, 3-ethyl-2-[7-(3-ethyl-2-benzoxazolidene)-1,3,5-heptatrienyl]-, iodide 3.135
- 4-Benzoylbenzimidazo[2,10*a*]benz[*d*]isoquinolin-7-one 3.10
- 5-Benzylamino-9-diethylaminobenzo[*a*]phenothiazinium 3.14
- 5-Benzylamino-9-diethylaminobenzo[*a*]phenoxazinium 3.22
- Bergapten 1.258
- Biacetyl 1.108
- Bicyclo[2.2.1]heptane-2,3-dione, 1,7,7-trimethyl- 1.109
- Bicyclo[2.2.1]heptane-2-thione 1.110
- Bicyclo[2.2.1]heptane-2-thione, 3,3-dimethyl- 1.111
- Bicyclo[2.2.1]heptane-2-thione, 1,3,3,7,7-pentamethyl- 1.112
- Bicyclo[2.2.1]heptane-2-thione, 1,3,3-trimethyl- 1.113
- Bicyclo[2.2.1]heptane-2-thione, 1,7,7-trimethyl- 1.114
- Biline-8,12-dipropanoic acid, 18-ethenyl-3-ethylidene-1,2,3,15,16,19,22,24-octahydro-2,7,13,17-tetramethyl-1,19-dioxo-, dimethyl ester 3.33
- Biphenyl 1.115
- (2,2'-Bipyridine)bis(bromo)platinum(II) 3.34
- (2,2'-Bipyridine)bis(chloro)platinum(II) 3.35
- (2,2'-Bipyridine)bis(cyano)platinum(II) 3.36
- (2,2'-Bipyridine)bis(iodo)platinum(II) 3.37
- (2,2'-Bipyridine)bis(thiocyanato)platinum(II) 3.38
- 2,2'-Bipyridine(2,3-naphthalenediolato)palladium(II) 3.39
- 2,2'-Bipyridine(2,3-naphthalenediolato)platinum(II) 3.40
- 2,2'-Biquinoline(2,3-naphthalenediolato)palladium(II) 3.41
- 2,2'-Biquinoline(2,3-naphthalenediolato)platinum(II) 3.42
- Bis(azido)(2,2'-bipyridine)palladium(II) 3.45
- Bis(azido)(2,2'-biquinoline)palladium(II) 3.43
- Bis(azido)(2,2'-biquinoline)platinum(II) 3.44
- Bis(azido)(4,7-diphenyl-1,10-phenanthroline)palladium(II) 3.46
- Bis(azido)(4,7-diphenyl-1,10-phenanthroline)platinum(II) 3.47
- Bis(azido)(1,10-phenanthroline)palladium(II) 3.48

- Bis(azido)(1,10-phenanthroline)platinum(II) 3.49  
 Bis(2,2'-bipyridine)bis(cyano)ruthenium(II) 1.116  
 6,7-Bis(2-carboxyethyl)-1,3,5,8-tetramethyl-2,4-diethenylporphineatodichlorotin(IV) ion 2.172  
 4,4'-Bis(dimethylamino)benzophenone 1.89  
 3,7-Bis(dimethylamino)phenothiazinium 1.245  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]selenopyrylium 3.184  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]selenopyran-4-ylidene]3-propenyl]pyrylium 3.159  
 2,6-Bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-4-(2-butenyl)]selenopyrylium 3.185  
 2,6-Bis(1,1-dimethylethyl)-4-[2-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-4-(2-pentenyl)]selenopyrylium 3.186  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]selenopyrylium 3.187  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]thiopyrylium 3.195  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]ethyl]telluropyrylium 3.191  
 2,6-Bis(1,1-dimethylethyl)-4-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]ethyltelluropyrylium 3.192  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]pyrylium 3.160  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]selenopyrylium 3.188  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]telluropyrylium 3.193  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxytelluropyran-4-ylidene]-3-propenyl]thiopyrylium 3.196  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxythiapyran-4-ylidene]-3-propenyl]pyrylium 3.161  
 2,6-Bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)-1,1-dihydroxythiopyran-4-ylidene]-3-propenyl]thiopyrylium 3.197  
 7,12-Bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropenoatocobaltate(III), dihydrogen 2.155  
 7,12-Bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropenoatomanganate(III), dihydrogen 2.159  
 7,12-Bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropenoic acid 2.154  
 7,12-Bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropenoic acid, dimethyl ester 2.158  
 Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthrolineosmium(II) 1.117  
 Bis(1,10-phenanthroline)-4,7-di(sulfonatophenyl)-1,10-phenanthrolineruthenium(II) 1.118  
 Bis(1,10-phenanthroline)[(1,10-phenanthroline-4,7-diylyl)bis[benzenesulfonato]]ruthenium(II) 1.118  
 Bis-porphyrin 2.148  
 1,5-Bis(2-thienyl)benzene 1.300  
 2,6-Bis(2-thienyl)pyridine 1.266  
 Bis(tri-*n*-hexyloxysiloxy)-2,3-naphthalocyaninatosilicon 2.11  
 2,3-Bornanedione 1.109  
 5-Bromo-2-(9-chloro-3-oxonaphtho[1,2-*b*]thien-2-ylidene)-4-methyl-1,2-dihydroindol-3-one 3.102  
 2-Bromochrysene 1.125  
*N*-[2-[(2-Bromo-6-cyano-4-nitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide 3.57  
*N*-[2-[(2-Bromo-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide 3.58  
 1-Bromonaphthalene 1.222  
 5-Bromo-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion 1.119  
 2-Bromo- $\alpha$ -terthienyl 1.286  
 2-[7-(4-Bromo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate 3.95  
 Buckminsterfullerene 1.120  
 Butanamide, 2-(4-methylphenylazo)-3-oxo-*N*-phenyl- 3.61  
 Butanamide, 3-oxo-*N*-phenyl-2-(phenylazo)- 3.62  
 2,3-Butanedione 1.108  
 9-*tert*-Butylanthracene 1.24  
 4-*tert*-Butylcatechol(1,10-phenanthroline)palladium(II) 3.50  
 Cadmium(II) chlorotexaphyrin nitrate 2.219  
 Cadmium(II) 7,12-diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.179  
 Cadmium(II) diphenyltetrabenzoporphyrin 2.215  
 Cadmium(II) mesoporphyrin IX, dimethyl ester 2.179  
 Cadmium(II) 2,3,7,8,12,13,17,18-octaethylporphyrin 2.74  
 Cadmium(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.118  
 Cadmium(II) tetraphenylporphyrin 2.137  
 Cadmium(II) texaphyrin nitrate 2.220  
*all-trans*-C<sub>17</sub> aldehyde 1.214  
*all-trans*-C<sub>22</sub> aldehyde 1.122  
 Caledon Brilliant Orange 6R 3.64  
 Caledon Brown R 3.75  
 Caledon Golden Orange G 3.147  
 Caledon Paper Gold Orange G 3.147  
 Camphorquinone 1.109  
 3-Carbethoxypseudosoralen 1.254  
 3-Carbethoxysoralen 1.256

- 4,4'-Carbocyanine, 1,1'-diethyl-, iodide 3.52  
 β-Carboline 1.226  
 Carbon seventy-atom molecule 1.121  
 Carbon sixty-atom molecule 1.120  
 9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylidene 3.165  
*N*-[9-(2-Carboxyphenyl)-6-(diethylamino)xanthen-3-ylidene]-*N*-ethylethanaminium 3.165  
 β-apo-14"-Carotenal 1.122  
 Catechol(1,10-phenanthroline)palladium(II) 3.53  
 Catechol(1,10-phenanthroline)platinum(II) 3.54  
 Cercosporin 1.234  
 Chalcogenopyrylium dye 1a 3.162  
 Chloranil 1.102  
 Chloranil/Anisole 1.103  
 Chloranil/Durene 1.104  
 Chloranil/Hexamethylbenzene 1.105  
 Chloranil/1,2,3-Trimethoxybenzene 1.106  
 Chlorin a<sub>6</sub> 2.200  
 Chlorin e<sub>6</sub> 2.200  
 Chloroaluminum(III) sulfophthalocyanine 2.29  
 Chloroaluminum(III) trisulfophthalocyanine 2.28  
 1-Chloroanthracene 1.14  
 9-Chloroanthracene 1.15  
 1-Chloroanthraquinone 1.47  
 2-Chloroanthraquinone 1.48  
 5-Chloro-2-[2-[3-[(5-chloro-3-ethyl-2-benzothiazolidene)ethylidene]-2-(diphenylamino)-1-cyclopenten-1-yl]ethenyl]-3-ethylbenzothiazolium, perchlorate 3.25  
 2-Chlorochrysene 1.126  
 4-Chloro-1,3-dihydroxybenzene 1.80  
 5-Chloro-1,3-dimethoxybenzene 1.74  
 2-Chloro-10-dimethylaminopropylphenothiazine 3.142  
 2-Chloro-*N,N*-dimethylphenothiazinc-10-propanamine 3.142  
*N*-[2-[(2-Chloro-4,6-dinitrophenyl)azo]-5-[(2-cyanoethyl)(2-hydroxyethyl)amino]-4-methoxyphenyl]acetamide 3.59  
 Chlorogallium(III) sulfophthalocyanine 2.36  
 Chlorogallium(III) tetrasulfophthalocyanine 2.35  
 Chlorogallium(III) trisulfophthalocyanine 2.36  
 Chlorohydroquinone 1.82  
 6-Chloro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate 3.26  
 5-Chloro-1,10-phenanthrolinebis(1,10-phenanthroline)ruthenium(II) ion 1.123  
 Chlorophyll *a* 2.3  
 Chlorophyll *b* 2.4  
 Chlorophyll (oil soluble) 2.5  
 4'-Chloropivalothiophenone 1.248  
*N*-[4-[(7-Chloro-4-quinolyl)amino]butyl]-5,10,15,20-tetraphenylporphine-2-propionamide 2.202  
 4-Chlororesorcinol 1.80  
 20-Chloro-5,9,10,14-tetraethyl-4,15-dimethyl-8,11-imino-6,3:13,16-dinitriolo-1,18-benzodiazacycloicosinatocadmium(II) nitrate 2.219  
 20-Chloro-5,9,10,14-tetraethyl-4,15-dimethyl-8,11-imino-6,3:13,16-dinitriolo-1,18-benzodiazacycloicosinatozinc(II) chloride 2.224  
 Chloro-2,9,16,23-[tetrakis(1,1-dimethylethyl)phthalocyaninato]aluminate(III) 2.42  
 2-[7-(4-Chloro-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate 3.96  
 Chlorpromazine 3.142  
 Chromium(III) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate 3.87  
 Chromium(III) 1-(2-hydroxyphenylazo)-2-naphtholate 3.123  
 Chrysene 1.124  
 Chrysene, 2-bromo- 1.125  
 Chrysene, 2-chloro- 1.126  
 C.I. 11855 3.56  
 C.I. 12120 3.130  
 C.I. 44045 3.107  
 C.I. 59100 3.65  
 C.I. 60700 1.46  
 C.I. 61200 3.6  
 C.I. 62015 1.59  
 C.I. 64500 1.65  
 C.I. 67300 3.5  
 C.I. 74240 2.45  
 Cibacron Rubine 4G-P 3.117  
 Cibacron Scarlet 4G-P 3.117  
 C.I. Reactive Red 16 3.117  
 C.I. Reactive Red 35 3.164  
 Cobalt, bis(cyano)[tetramethyl-12,13-didehydro-2,18-bis(2-methoxy-2-oxoethyl)-3,5,8,8,13,15,18,19-octamethyl-3,7,12,17-corrintetrapropanoato- 3.55  
 Cobalt(II) bis[1-(2-hydroxyphenylazo)-2-naphtholate] 3.124  
 Cobalt(III) bis[1-(2-hydroxyphenylazo)-2-naphtholate] 3.125  
 Cobalt(II) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate 3.85  
 Cobalt(III) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate 3.86  
 Cobalt(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate 3.91  
 Cobalt(III) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate 3.92  
 Cobalt(III) hematoporphyrin 2.155

- Cobalt(II) mesoporphyrin IX dimethanesulfonate-6,7-dimethylaminopropyl derivative 2.50
- Cobalt(II) sulfophthalocyanine 2.32
- Cobalt(III) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.119
- Cobalt(II) 1,3,5,8-tetramethyl-2,4-diethyl-6,7-di(3-dimethylaminopropyl)porphyrin, dimethanesulfonate 2.50
- Cobalt(II) 5,10,15,20-tetraphenylporphyrin 2.139
- Cobrynic acid, bis(cyano)-7-de(carboxymethyl)-7,8-didehydro-, hexamethyl ester 3.55
- Copper(II), 2,11,20,29-tetrakis(1,1-dimethylethyl)tetranaphtho[2,3-*b*:2',3'-*g*:2'',3''-*l*:2''',3'''-*q*]porphyrinato- 2.10
- Copper(II) 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid 2.156
- Copper(II) 2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate 3.88
- Copper(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate 3.93
- Copper(II) hematoporphyrin IX 2.156
- Copper(II) 1-(2-hydroxyphenylazo)-2-naphtholate 3.126
- Copper(II) mesoporphyrin IX, dimethyl ester 2.180
- Copper(II) 2,3,7,8,12,13,17,18-octaethyl-5-methylporphyrin 2.86
- Copper(II) 2,3,7,8,12,13,17,18-octaethylporphyrin 2.75
- Copper(II) sulfophthalocyanine 2.33
- Copper(II) 2,11,20,29-tetra-*tert*-butylnaphthalocyanine 2.10
- Copper(II) 2,9,16,23-tetra-*tert*-butylphthalocyanine 2.43
- Copper(II) tetracarboxyphthalocyanine 2.40
- Copper(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.120
- Copper(II) tetraphenylporphyrin 2.140
- Copper(II) 5,10,15,20-tetraphenylporphyrin 2.140
- Coproporphyrin I 2.204
- [22]Coproporphyrin II 2.6
- Coproporphyrin III 2.205
- Coproporphyrin III, tetramethyl ester 2.206
- Coproverdin II trimethyl ester 2.229
- Coronene 1.127
- Coumarin 1.128
- Coumarin 1 1.129
- Coumarin 102 1.99
- Coumarin 460 1.129
- Coumarin 47 1.129
- Coumarin, 7-(diethylamino)-4-methyl- 1.129
- Cryptocyanine 3.52
- 4'-Cyanoacetophenone 1.3
- 9-Cyanoanthracene 1.16
- N*-[5-(2-Cyanoethyl)(2-hydroxyethyl)amino]-2-[(2,4-dinitrophenyl)azo]-4-methoxyphenyl]acetamide 3.60
- 2-Cyano- $\alpha$ -terthienyl 1.287
- Cycloheptatriene 1.130
- 1,3-Cyclohexadiene 1.131
- 2-Cyclohexenethione, 3,5,5-trimethyl- 1.132
- Cyclomycin 3.108
- Cyclopentadiene 1.133
- Daunomycin 3.109
- Daunomycinone 3.110
- Daunorubicin 3.109
- 7-Dehydrocholesterol 1.134
- Deuteroporphyrin-*d*<sub>2</sub>, dimethyl ester 2.199
- Deuteroporphyrin, dimethyl ester 2.198
- Deuteroporphyrin IX 2.197
- Deuteroverdin methyl ester 2.228
- Diacenaphtho[1,2-*b*:2',1'-*d*]thiophene 1.135
- Diacyetyl 1.108
- 3,6-Diaminoacridine 1.9
- 1,2-Diaminoanthraquinone 1.49
- 1,4-Diaminoanthraquinone 1.50
- 1,5-Diaminoanthraquinone 1.51
- 1,8-Diaminoanthraquinone 1.52
- 2,6-Diaminoanthraquinone 1.53
- 1,5-Diamino-2-bromo-4,8-dihydroxyanthraquinone 1.54
- 1,5-Diamino-4,8-dihydroxyanthraquinone 1.55
- 1,8-Diamino-4,5-dihydroxyanthraquinone 1.56
- 2,5-Diamino-1,8-dihydroxyanthraquinone 1.57
- 2,7-Diamino-1,8-dihydroxyanthraquinone 1.58
- 4,5-Diamino-1,8-dihydroxyanthraquinone 1.56
- 3,7-Diamino-2,8-dimethyl-5-phenylphenazinium 3.183
- 1,4-Diamino-2-methoxyanthraquinone 1.59
- 3,6-Diamino-10-methylacridinium 1.10
- 3,7-Diaminophenothiazinium 1.246
- 1,4-Diamino-[4-(phenylaminosulfonyl)phenoxy]anthraquinone 1.60
- 1,4-Diazanaphthalene 1.270
- 2,7-Diazapyrene, 2,7-dimethyl- 1.136
- Diazene, 1-(4-acetylamino-5-hydroxy-2-methylphenyl)-2-phenyl- 3.56
- Diazene, 1-(2-bromo-6-cyano-4-nitrophenyl)-2-[2-(acetylamino)-4-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-5-methoxyphenyl]- 3.57
- Diazene, 1-(2-bromo-4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-5-methoxyphenyl]- 3.58
- Diazene, 1-(2-chloro-4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-5-methoxyphenyl]- 3.59
- Diazene, 1-(4,6-dinitrophenyl)-2-[2-(acetylamino)-4-[*N*-(2-cyanoethyl)-*N*-(2-hydroxyethyl)amino]-5-methoxyphenyl]- 3.60
- Diazene, 1-(4-methylphenyl)-2-[1-(phenylaminocarbonyl)-2-oxopropyl]- 3.61
- Diazene, 1-phenyl-2-[1-(phenylaminocarbonyl)-2-oxopropyl]- 3.62

- 1,2,7,8-Dibenzanthanthrene 1.262  
 1,2,5,6-Dibenzanthracene 1.137  
 Dibenz[*a,h*]anthracene 1.137  
 Dibenzanthrone 3.1  
 Dibenz[*f,i,j*]isoquinoline-2,7-dione, 3-methyl-6-(phenylamino)- 3.63  
 Dibenzo[3,4;5,6][2]benzopyrano[7,8,1-*mna*]xanthene 1.37  
 Dibenzo[*def,mno*]chrysene 1.138  
 Dibenzo[*b,def*]chrysene-7,14-dione 3.65  
 Dibenzo[*def,mno*]chrysene-6,12-dione, 4,10-dibromo- 3.64  
 Dibenzo[*a,o*]perylene 1.213  
 Dibenzo[*a,o*]perylene, 7,16-diphenyl- 1.139  
 Dibenzo[*aj*]perylene-8,16-dione 1.215  
 2,3:7,8-Dibenzopyrene-1,6-dione 3.65  
 2,3:7,8-Dibenzopyrene-1,6-dione, 4,9-dibromo- 3.66  
 2,3:7,8-Dibenzopyrene-1,6-dione, 4,9-dichloro- 3.67  
 2,3,7,8-Dibenzopyrene-1,6-quinone 3.65  
 4,5'-Dibenzoylaminanthrimide 3.75  
 11,12-Dibenzoyl-9,10-dihydro-9,10-dimethoxy-9,10-ethenoanthracene 1.144  
 11,12-Dibenzoyl-9,10-dihydro-9,10-ethenoanthracene-9-carbonitrile 1.148  
 11,12-Dibenzoyl-9,10-dihydro-9,10-ethenoanthracene-9-carboxaldehyde 1.149  
 11,12-Dibenzoyl-9,10-dihydro-9-hydroxy-9,10-ethenoanthracene 1.145  
 11,12-Dibenzoyl-9,10-dihydro-9-methoxy-9,10-ethenoanthracene 1.146  
 11,12-Dibenzoyl-9-ethyl-9,10-dihydro-9,10-ethenoanthracene 1.147  
 4,10-Dibromoanthrone 3.64  
 9,10-Dibromoanthracene 1.17  
 4,10-Dibromodibenzo[*def,mno*]chrysene-6,12-dione 3.64  
 4,9-Dibromo-2,3:7,8-dibenzopyrene-1,6-dione 3.66  
 Dibromo-16,17-dimethoxyviolanthrone 3.2  
 4',5'-Dibromo-2',7'-dinitrofluorescein dianion 1.156  
 Dibromofluorescein dianion 1.155  
 Dibromo(1,10-phenanthroline)platinum(II) 3.68  
 2,9-Dibromo- $\alpha$ -terthienyl 1.288  
 Di-*tert*-butylthioketone 1.229  
 6,15-Dichloroantra[9,1,2-*cde*]benzo[*rsr*]pentaphene-10,18-dione 3.4  
 9,10-Dichloroanthracene 1.18  
 4,4'-Dichlorobenzil 1.84  
 4,9-Dichloro-2,3:7,8-dibenzopyrene-1,6-dione 3.67  
 2',7'-Dichlorofluorescein dianion 1.158  
 4',5'-Dichlorofluorescein dianion 1.159  
 5,5'-Dichloro-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide 3.198  
 6,15-Dichloroisoviolanthrone 3.4  
 Dichloro(1,10-phenanthroline)platinum(II) 3.69  
 Dichloro[5,10,15,20-tetrakis(4-sulfonatophenyl)porphinatostannate(IV) ion 2.131  
 Dichloro(5,10,15,20-tetraphenylporphinato)tin(IV) 2.141  
 Dichlorotin(IV) protoporphyrin 2.172  
 9,10-Dicyanoanthracene 1.19  
 Dicyanobis(1,10-phenanthroline)ruthenium(II) 1.140  
 4-(Dicyanomethylene)-2-methyl-6-(*p*-dimethylaminostyryl)pyran 3.146  
 Dicyano(1,10-phenanthroline)platinum(II) 3.70  
 3,4-Didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoatomagnesate, hydrogen 2.20  
 21,23-Dideutero-7,12-diethenyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.167  
 21,23-Dideutero-2,3,7,8,12,13,17,18-octaethylporphine 2.54  
 7,12-Diethenyl-3,8,13,17-tetramethylporphine-2,18-dipropanoatozincate(II) 2.173  
 7,12-Diethenyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid 2.165  
 7,12-Diethenyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.166  
 7-(Diethylamino)-4-methylcoumarin 1.129  
 4-(4'-Diethylamino-2'-methylphenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one 3.154  
 4-(4'-Diethylaminophenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one 3.156  
 1,1'-Diethyl-4,4'-carbocyanine iodide 3.52  
 Diethyl ketone 1.231  
 3,3'-Diethyl-2,2'-oxatricarbocyanine iodide 3.135  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoatopalladium(II)-2,18-dipropanoic acid, dimethyl ester 2.183  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoatocuprate(II), dimethyl ester 2.180  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoatomagnesiate(II), dimethyl ester 2.181  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoatozincate(II), dimethyl ester 2.185  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, diethyl ester 2.176  
 7,12-Diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.177  
 3,3'-Diethyl-2,2'-thiatricarbocyanine iodide 3.194  
 5,5'-Difluoro-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide 3.199  
 7,12-Diformyldeuteroporphyrin IX dimethyl ester 2.188  
 Dihematoporphyrin ester 3.71  
 Dihematoporphyrin ester chlorin 3.72  
 2,4-Dihydro-2-(4-bromophenyl)-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamylpyrazol-3-one 3.150

- 2,4-Dihydro-2-(4-chlorophenyl)-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamylpyrazol-3-one 3.151
- 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(3-methoxyphenyl)pyrazol-3-one 3.152
- 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(3-methylphenyl)pyrazol-3-one 3.153
- 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methylcarbamyl-2-(2,4,6-trichlorophenyl)pyrazol-3-one 3.155
- 2,4-Dihydro-4-(4-diethylamino-2-methylphenyl)imino-5-methyl-2-phenylpyrazol-3-one 3.154
- 2,4-Dihydro-4-(4-diethylaminophenyl)imino-5-methyl-2-phenylpyrazol-3-one 3.156
- (9,10-Dihydro-9,10-dimethoxy-9,10-ethenoanthracene-11,12-diyl)bis[phenylmethanone] 1.144
- 2,4-Dihydro-4-(4-dimethylaminophenyl)imino-5-methyl-2-phenylpyrazol-3-one 3.157
- 1,4-Dihydro-1-ethyl-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylate ion 3.134
- 1,4-Dihydro-1-ethyl-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid 3.133
- (9,10-Dihydro-9-hydroxy-9,10-ethenoanthracene-11,12-diyl)bis[phenylmethanone] 1.145
- (9,10-Dihydro-9-methoxy-9,10-ethenoanthracene-11,12-diyl)bis[phenylmethanone] 1.146
- 2,3-Dihydro-2-methyl-1,2-benzothiazin-4-one 1,1-dioxide 3.24
- 3,4-Dihydro-1-naphthalenone 1.292
- 1,2-Dihydroxyanthraquinone 1.61
- 1,8-Dihydroxyanthraquinone 1.62
- 1,8-Dihydroxy-9-anthrone 1.68
- 1,8-Dihydroxy-9-anthrone, conjugate base 1.69
- 1,3-Dihydroxybenzene 1.79
- 1,4-Dihydroxybenzene 1.81
- 3',6'-Dihydroxyspiro[isobenzofuran-1,9'-xanthen]-3-one, ion(1-) 1.154
- Diodofluorescein dianion 1.160
- Diodo(1,10-phenanthroline)platinum(II) 3.73
- 4,5-Diiodosuccinylfluorescein dianion 1.311
- Diisopropyl ketone 1.232
- 3,4-Dimercaptotoluene(1,10-phenanthroline)palladium(II) 3.74
- 4,4'-Dimethoxybenzil 1.85
- 4,4'-Dimethoxybenzophenone 1.90
- (Z)-2,18-Di(methoxycarbonylethyl)-7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethylporphinatotin(IV) 2.192
- (Z)-2,18-Di(methoxycarbonylethyl)-7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethylporphinatozinc(II) 2.193
- 1,4-Dimethoxy-9,10-diphenylanthracene 1.20
- 2,4-Di( $\alpha$ -methoxyethyl)deuteroporphyrin dianion 2.164
- 5,5'-Dimethoxy-1,1',3,3,3',3'-hexamethyltricarbocyanine, iodide 3.200
- 5,8-Dimethoxypsoralen 1.257
- 4,4'-Dimethoxythiobenzophenone 1.293
- 4,7-Dimethylallopsoralen 1.194
- 4-(4'-Dimethylaminophenyl)imino-3-methyl-1-phenyl-2-pyrazolin-5-one 3.157
- N*-[4-[(4-Dimethylamino)phenyl]phenylmethylene]-2,5-cyclohexadiene-1-ylidine]-*N*-methylmethaminium 3.103
- 4,4'-Dimethylangelicin 1.200
- 4,5'-Dimethylangelicin 1.199
- 4',5-Dimethylangelicin 1.201
- 6,4-Dimethylangelicin 1.198
- 6,4'-Dimethylangelicin 1.202
- 9,10-Dimethylanthracene 1.21
- N,N'*-Dimethylanthra[2,1,0-def:6,5,10-d'e'f']diisoquinoline 1.38
- 9,10-Dimethylbenz[a]anthracene 1.73
- 3,3-Dimethylbicyclo[2.2.1]heptane-2-thione 1.111
- (E)-2-(3,3-Dimethyl-1-but enyl)anthracene 1.22
- (Z)-2-(3,3-Dimethyl-1-but enyl)anthracene 1.23
- N,N'*-Dimethyl-2,7-diazapyrene 1.136
- (Z)-Dimethyl 7-[2-(dimethylamino)-2-oxoethyl]-8-ethyl-7,8-dihydro-3,7,12,17-tetramethylporphine-2,18-dipropionate 2.189
- (Z)-Dimethyl 7-[2-(dimethylamino)-2-oxoethyl]-8-ethylidene-7,8-dihydro-3,7,12,17-tetramethylporphine-2,18-dipropionate 2.190
- (Z)-Dimethyl 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethylporphine-2,18-dipropionate 2.191
- 2,2'-Dimethyl-4,4',5,5',7,7'-hexahydroxymesonaphthodianthrone 1.238
- 1,1-Dimethyl-2-naphthalenethione 1.224
- 2,6-Dimethyl-2,4,6-octatriene 1.228
- 2,4-Dimethyl-3-pentanone 1.232
- 2,2-Dimethyl-1-phenyl-1-propanethione 1.247
- 1,3-Dimethylpyrazolo[1',2':2,3][1,2,3]triazolo[4,5- $\alpha$ ]phenazin-4-i um 3.158
- Dimethyl 3,7,12,17-tetramethylporphine-2,18-dipropanoate 2.198
- 3,3-Dimethylthiocamphor 1.112
- 3,6-Dimethyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate 3.27
- 1,8-Dinaphthalene thiophene 1.135
- Dinaphtho[2,3:*a*:2',3'-*i*]carbazole-4,9-diamine, *N,N'*-dibenzoyl-10,15,16,17-tetrahydro-5,10,15,17-tetraoxo- 3.75

|  |       |   |  |
|--|-------|---|--|
| 5,10-Dinitroetioporphyrin I  | 2.95  | 9,10-Ethenoanthracene, 9-acetoxy-11,12-dibenzoyl-9,10-dihydro-                                      | 1.143  |
| 5,15-Dinitroetioporphyrin I  | 2.97  | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-  | 9,10-dimethoxy- 1.144                          |
| 16,17-Dinitroviolanthrone  | 3.3   | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-9-hydroxy-                                      | 1.145  |
| 1,8-Diphenylanthra[2,1-d:6,5-d']bisthiazole-6,12-dione                   | 3.5   | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9,10-dihydro-9-methoxy-                                      | 1.146  |
| 9,10-Diphenylanthracene  | 1.25  | 9,10-Ethenoanthracene, 11,12-dibenzoyl-9-ethyl-9,10-dihydro-  | 1.147  |
| 2,5-Diphenyl-3,4-benzofuran  | 1.219 | 9,10-Ethenoanthracene-9-carbonitrile, 11,12-dibenzoyl-9,10-dihydro-                                 | 1.148  |
| 2,3-Diphenyl-1-benzopyran-4-one  | 1.96  | 9,10-Ethenoanthracene-9-carboxaldehyde, 11,12-dibenzoyl-9,10-dihydro-                               | 1.149  |
| 2,6-Diphenyl-1,4-benzoquinone  | 1.100 | 2-Ethenylanthracene   | 1.34   |
| 2,6-Diphenyl-1,4-benzoquinone/Triphenylamine                             | 1.101 | 9-Ethenyl-14-ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-3-phorbinepropanoic acid, | 3,7,11,15-tetramethyl-2-hexadecenyl ester 2.13 |
| 2,3-Diphenylchromone   | 1.96  | 9-Ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoic acid,      | 3,7,11,15-tetramethyl-2-hexadecenyl ester 2.12 |
| 1,6-Diphenyl-1,3,5-hexatriene  | 1.216 | 7(12)-Ethenyl-12(7)-formyldeuteroporphyrin IX dimethyl ester  | 2.194  |
| 1,3-Diphenylisobenzofuran  | 1.219 | 7-Ethenyl-12-(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid                   | 2.195  |
| 1,8-Diphenyl-1,3,5,7-octatetraene  | 1.227 | 9-[2-(Ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethylxanthylum                              | 3.166  |
| (4,7-Diphenyl-1,10-phenanthroline)bis(1,10-phenanthroline)osmium(II) ion | 1.141 | (9-Ethyl-9,10-dihydro-9,10-ethenoanthracene-11,12-diyi)bis[phenylmethanone]                         | 1.147  |
| 4,7-Diphenyl-1,10-phenanthroline(2,3-naphthalenediolato)platinum(II)     | 3.76  | 3-Ethyl-2-[7-(3-ethyl-2-benzothiazolylidene)-1,3,5-heptatrienyl]benzothiazolium iodide              | 3.194  |
| 3,4-Diphenylsydnone  | 1.280 | 3-Ethyl-2-[7-(3-ethyl-2-benzoxazolylidene)-1,3,5-heptatrienyl]benzoxazolium iodide                  | 3.135  |
| 6,13-Diphenyltetrabenzo[b,g,l,q]porphinatocadmium(II)                    | 2.215 | 1-Ethyl-4-[3-(1-ethyl-4-quinolinylidene)-1-propenyl]quinolinium iodide                              | 3.52   |
| 6,13-Diphenyltetrabenzo[b,g,l,q]porphinatomagnesium(II)                  | 2.216 | Etioporphyrin- <i>d</i> <sub>2</sub>  | 2.61   |
| 6,13-Diphenyltetrabenzo[b,g,l,q]porphinatozinc(II)                       | 2.217 | Etioporphyrin I   | 2.93   |
| 2,5-Diphenylthiophene  | 1.296 | Europium(III) dimethyltexaphyrin dihydroxide  | 2.221  |
| 9,18-Diphenyltribenzo[a,f,j]perylene                                     | 1.303 | Flavine mononucleotide  | 1.275  |
| Disperse Bluc 1  | 1.65  | Flavone   | 1.98   |
| Disperse bright pink   | 1.59  | Flavone, 3-hydroxy-   | 1.97   |
| Disperse Orange  | 1.46  | Fluoranthene  | 1.150  |
| Disperse Orange 11   | 1.46  | Fluorene  | 1.151  |
| Disperse Polyester Yellow 4Z   | 3.10  | Fluorene, 9-(phenylsulfonyl)-, ion(1-)  | 1.152  |
| Disperse Red 11  | 1.59  | Fluoren 9 one   | 1.153  |
| Disperse red 2S  | 1.43  | 9-Fluorenone  | 1.153  |
| Disperse violet K  | 1.50  | Fluorescein, 2',7'-dibromo-4'-(hydroxymercuri)-, disodium salt                                      | 1.157  |
| Disperse Yellow 3  | 3.56  | Fluorescein, 2',4',5',7'-tetrabromo-, methyl ester  | 1.164  |
| 1,3-Di(2-thienyl)benzene   | 1.299 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, 6-O-acetyl-, ethyl ester                   | 1.170  |
| 2,5-Di(2-thienyl)furan   | 1.192 | Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester                               | 1.171  |
| Doxorubicin  | 3.111 |   |  |
| Duroquinone  | 1.107 |   |  |
| Eosin, methyl ester  | 1.164 |   |  |
| Eosin B dianion  | 1.156 |   |  |
| Eosin dianion  | 1.161 |   |  |
| Eosin monoanion, benzyl ester  | 1.162 |   |  |
| Eosin monoanion, <i>p</i> isopropylbenzyl ester                          | 1.163 |   |  |
| Eosin monoanion, methyl ester  | 1.165 |   |  |
| Ergosta-5,7,22-trien-3-ol (3β)   | 1.142 |   |  |
| Ergosterol   | 1.142 |   |  |
| Erythrosin dianion   | 1.190 |   |  |
| Ethanedione, bis(4-chlorophenyl)-  | 1.84  |   |  |
| Ethanedione, bis(2,4,6-trimethylphenyl)-                                 | 1.86  |   |  |
| Ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethylporphine)]              | 2.68  |   |  |

- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, benzyltriphenylphosphonium salt 1.173
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, diphenyliodonium salt 1.174
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, diphenylmethylsulfonium salt 1.175
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, triethylammonium salt 1.176
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester, 2,4,6-triphenylpyrylium salt 1.177
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(benzyltriphenylphosphonium) salt 1.178
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(diphenyliodonium) salt 1.179
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, bis(triethylammonium) salt 1.180
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, complexed with dicyclohexyl-18-crown-8 1.181
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, ethyl ester 1.182
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, ethyl ester, triethylammonium salt 1.183
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, *p*-isopropylbenzyl ester 1.184
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, *O*-methyl-, methyl ester 1.186
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, methyl ester 1.187
- Fluorescein, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, octyl ester, tributylammonium salt 1.189
- Fluorescein, 4,5,6,7-tetrachloro-2',4',5',7'-tetraiodo-, lactone 1.168
- Fluorescein, 2,4,5,7-tetraiodosuccinyl-, bound as copoly(styrene-*p*-vinylbenzyl ester) 3.207
- Fluorescein, 2,4,5-triiodosuccinyl-, bound as copoly(styrene-*p*-vinylbenzyl ester) 3.208
- Fluorescein dianion 1.154
- Fluorescein dianion, dibromo- 1.155
- Fluorescein dianion, 4',5'-dibromo-2',7'-dinitro- 1.156
- Fluorescein dianion, 2',7'-dichloro- 1.158
- Fluorescein dianion, 4',5'-dichloro- 1.159
- Fluorescein dianion, diiodo- 1.160
- Fluorescein dianion, 2',4',5',7'-tetrabromo- 1.161
- Fluorescein dianion, 2',4',5',7'-tetrabromo-3,4,5,6-tetrachloro- 1.166
- Fluorescein dianion, 2',4',5',7'-tetrachloro- 1.167
- Fluorescein dianion, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo- 1.169
- Fluorescein dianion, 2',4',5',7'-tetraiodo- 1.190
- Fluorescein dianion, tribromo- 1.191
- Fluorescein monoanion, 2',4',5',7'-tetrabromo-, benzyl ester 1.162
- Fluorescein monoanion, 2',4',5',7'-tetrabromo-, *p*-isopropylbenzyl ester 1.163
- Fluorescein monoanion, 2',4',5',7'-tetrabromo-, methyl ester 1.165
- Fluorescein monoanion, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, benzyl ester 1.172
- Fluorescein monoanion, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, *p*-isopropylbenzyl ester 1.185
- Fluorescein monoanion, 3,4,5,6-tetrachloro-2',4',5',7'-tetraiodo-, methyl ester 1.188
- 4-Fluorobenzophenone 1.91
- 6-Fluoro-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-iodo-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate 3.28
- 4'-Fluoropivalothiophenone 1.249
- N*-Formylkynurenine 1.76
- 5-Formyloctaethylporphyrin 2.150
- 5-Formyloctaethylporphyrin-*d*<sub>2</sub> 2.149
- 7(12)-Formyl-12(7)-vinyldeuteroporphyrin IX dimethyl ester 2.194
- Fulvic acids 3.77
- Furan, 2,5-di(2-thienyl)- 1.192
- Furo[2,3-*g*][1]benzopyran-7-carboxylic acid, 6-oxo-, ethyl ester 1.254
- Furo[3,2-*g*][1]benzopyran-6-carboxylic acid, 7-oxo-, ethyl ester 1.256
- Furo[2,3-*f*][1]benzopyran-7-one 1.11
- Furo[2,3-*f*][1]benzopyran-7-one, 8-acetyl- 1.193
- Furo[2,3-*f*][1]benzopyran-7-one, 4,9-dimethyl- 1.194
- Furo[2,3-*f*][1]benzopyran-7-one, 2,4,9-trimethyl- 1.195
- Furo[2,3-*f*][1]benzopyran-7-one, 3,4,9-trimethyl- 1.196
- Furo[2,3-*g*][1]benzopyran-6-one 1.253
- Furo[2,3-*h*][1]benzopyran-2-one 1.12
- Furo[2,3-*h*][1]benzopyran-2-one, 3-acetyl- 1.197
- Furo[2,3-*h*][1]benzopyran-2-one, 4,6-dimethyl- 1.198
- Furo[2,3-*h*][1]benzopyran-2-one, 4,8-dimethyl- 1.199
- Furo[2,3-*h*][1]benzopyran-2-one, 4,9-dimethyl- 1.200
- Furo[2,3-*h*][1]benzopyran-2-one, 5,9-dimethyl- 1.201
- Furo[2,3-*h*][1]benzopyran-2-one, 6,9-dimethyl- 1.202
- Furo[2,3-*h*][1]benzopyran-2-one, 4-methyl- 1.203
- Furo[2,3-*h*][1]benzopyran-2-one, 5-methyl- 1.204
- Furo[2,3-*h*][1]benzopyran-2-one, 8-methyl- 1.205
- Furo[2,3-*h*][1]benzopyran-2-one, 9-methyl- 1.206
- Furo[2,3-*h*][1]benzopyran-2-one, 4,6,9-trimethyl- 1.207
- Furo[3,2-*f*][1]benzopyran-7-one 1.208
- Furo[3,2-*f*][1]benzopyran-7-one, 8-acetyl- 1.209
- Furo[3,2-*g*][1]benzopyran-7-one 1.255
- Furo[3,2-*g*][1]benzopyran-7-one, 2-acetyl-5,9-dimethyl- 1.210
- Furo[3,2-*g*][1]benzopyran-7-one, 2-acetyl-9-methyl- 1.211
- Furo[3,2-*g*][1]benzopyran-7-one, 4,9-dimethoxy- 1.257
- Furo[3,2-*g*][1]benzopyran-7-one, 4-methoxy- 1.258
- Furo[3,2-*g*][1]benzopyran-7-one, 9-methoxy- 1.260
- Furo[3,2-*g*][1]benzopyran-7-one, 2,5,9-trimethyl- 1.261

- Furo[3,2-*h*][1]benzopyran-8-one 1.252  
 Furo[3,2-*h*][1]benzopyran-8-one, 7-acetyl- 1.212  
 Gallium(II) 5,10,15,20-tetraphenylporphyrin 2.142  
 Gilvocarcin V 3.11  
 Helianthrene 1.213  
 Hematoporphyrin, dimethyl ether, dianion 2.164  
 Hematoporphyrin derivative 3.78  
 Hematoporphyrin diacetate 2.157  
 Hematoporphyrin dimers 3.79  
 Hematoporphyrin dimethyl ester 2.158  
 Hematoporphyrin IX 2.154  
 Hematoporphyrin monomer:dimer:oligomer 2:3:9 3.80  
 Hematoporphyrin monomer:dimer:oligomer 4:2:1 3.81  
 Hematoporphyrin monomer:dimer:oligomer 5:3:4 3.82  
 Hematoporphyrin oligomers 3.83  
*(E,E,E)-2,4,6-Heptatrienal, 5-methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)-* 1.214  
 Heterocoerdianthrone 1.215  
 3,8,12,13,17,22-Hexaethyl-2,7,18,23-tetramethylsapphyrin, diprotonated 2.213  
 2,2',4,4',6,6'-Hexamethylbenzil 1.86  
 Hexamethyl Co $\alpha$  Co $\beta$ -dicyano-7-de(carboxymethyl)-7,8-didehydrocobyminate 3.55  
 1,1',3,3,3',3'-Hexamethylindotricarbocyanine iodide 3.202  
 1,1',3,3,3',3'-Hexamethylindotricarbocyanine perchlorate 3.203  
 1,1',3,3,3',3'-Hexamethyltricarbocyanine, fluoride 3.201  
 1,1',3,3,3',3'-Hexamethyltricarbocyanine, iodide 3.202  
 1,1',3,3,3',3'-Hexamethyltricarbocyanine, perchlorate 3.203  
 1,6-Hexanediylbis[3,8,12,17-tetramethyl-2,7,18-tris(2-carboxyethyl)porphine 2.207  
 1,3,5-Hexatriene, 1,6-diphenyl- 1.216  
 Humic acids 3.84  
 Hydroquinone 1.81  
 Hydroquinone, chloro- 1.82  
 1-Hydroxyanthraquinone 1.63  
 2-Hydroxyanthraquinone 1.64  
 Hydroxyethylvinyldeuteroporphyrin 2.195  
 3-Hydroxyflavone 1.97  
 3-Hydroxykynurenone 1.77  
*N*-[4-[(2-Hydroxy-5-methylphenyl)azo]phenyl]acetamide 3.56  
 4-Hydroxy-2-methyl-*N*-(2-pyridyl)-1,2-benzothiazine-3-carboxamide 1,1-dioxide 3.23  
*N*-[5-Hydroxy-8-[[2-(methylsulfonyl)-4-nitrophenyl]azo]-1-naphthalenyl-1,3-benzenedisulfonamide, conjugate base 3.120  
 4-Hydroxyquinoline-2-carboxylic acid 1.269  
 Hypericin 1.238  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, chromium(III) salt 3.87  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, cobalt(II) salt 3.85  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, cobalt(III) salt 3.86  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, copper(II) salt 3.88  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, iron(III) salt 3.89  
 Imidazole, 4,5-diphenyl-2-[(2-carboxy-5-methylphenyl)azo]-, nickel(II) salt 3.90  
 Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, cobalt(II) salt 3.91  
 Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, cobalt(III) salt 3.92  
 Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, copper(II) salt 3.93  
 Imidazole, 4,5-diphenyl-2-[(2-hydroxy-5-nitrophenyl)azo]-, nickel(II) salt 3.94  
 5-Iminodaunomycin 3.112  
 Indium(II) octaethylporphyrin 2.77  
 Indole, 1-methyl 1.217  
 Indolium, 2-[7-(4-bromo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate 3.95  
 Indolium, 5-chloro-1-[7-(5-chloro-1,3-dihydro)-1,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, iodide 3.198  
 Indolium, 2-[7-(4-chloro-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate 3.96  
 Indolium, 1-[7-(1,3-dihydro)-1,3,3,5-tetramethylindol-2-ylidene]-1,3,5-heptatrienyl]-, iodide 3.204  
 Indolium, 1-[7-(1,3-dihydro)-1,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, fluoride 3.201  
 Indolium, 1-[7-(1,3-dihydro)-1,3,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, iodide 3.202  
 Indolium, 1-[7-(1,3-dihydro)-1,3,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, perchlorate 3.203  
 Indolium, 5-fluoro-1-[7-(5-fluoro-1,3-dihydro)-1,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, iodide 3.199  
 Indolium, 2-[7-(4-iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, iodide 3.97  
 Indolium, 2-[7-(4-iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate 3.98  
 Indolium, 5-methoxy-1-[7-(5-methoxy-1,3-dihydro)-1,3,3-trimethylindol-2-ylidene]-1,3,5-heptatrienyl]-, iodide 3.200  
 Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-(2,2-dimethoxyethyl)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, tetrafluoroborate 3.99

- Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-(1-piperidinio)-1,3,5-heptatrienyl]-1,3,3-trimethyl-, bis(tetrafluoroborate) 3.100
- Indolium, 2-[7-(1,3,3-trimethyl-2-indol-2-ylidene)-1-[4-[3-(1,3,3-trimethyl-2-indolylidene)-2-propenyl]-1,3,5-heptatrienyl]-1,3-trimethyl-, tetrafluoroborate 3.101
- Indol-3-one, 5-bromo-2-(9-chloro-3-oxonaphtho[1,2-*b*]thien-2-ylidene)-4-methyl-1,2-dihydro- 3.102
- Ingrain Blue 1 2.45
- 2-[7-(4-Iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, iodide 3.97
- 2-[7-(4-Iodo-1,3,3-trimethyl-2-indol-2-ylidene)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, tetrafluoroborate 3.98
- $\beta$ -Ionone 1.218
- IR 140 3.25
- Iridium(III) tris(2,2'-bipyridine) 1.305
- Iron(III) bis[2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate] 3.89
- Iron(III) 1-(2-hydroxyphenylazo)-2-naphtholate 3.127
- Iron(II) sulfophthalocyanine 2.34
- Iron(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.121
- Iron(III) 5,10,15,20-tetraphenylporphyrin 2.143
- Isobenzofuran, 1,3-diphenyl- 1.219
- Isohematoporphyrin 2.163
- Isopimpinellin 1.257
- Isopseudopsoralen 1.208
- Isopsoralen 1.12
- Kryptocyanine 3.52
- Kynurenic acid 1.269
- Kynurenine 1.78
- Lead(II) 2,3,7,8,12,13,17,18-octaethylporphyrin 2.76
- Magnesium(II) diphenyltetrazenophosphoryn 2.216
- Magnesium(II) mesoporphyrin IX, dimethyl ester 2.181
- Magnesium(II) phthalocyanine 2.24
- Magnesium(II) protoporphyrin 2.170
- Magnesium(II) protoporphyrin, dimethyl ester 2.168
- Magnesium(II) 2,9,16,23-[tetrakis(1,1-dimethylethyl)phthalocyanine] 2.44
- Magnesium(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.123
- Magnesium(II) 3,8,15,17-tetramethyl-7,12-diethenylporphine-2,18-dipropanoic acid 2.170
- Magnesium(II) 3,8,15,17-tetramethyl-7,12-diethenylporphine-2,18-dipropanoic acid, dimethyl ester 2.168
- Malachite Green cation 3.103
- Manganese(III) hematoporphyrin 2.159
- Manganese(II) mesoporphyrin IX dimethanesulfonate-6,7-di(methylaminopropyl) derivative 2.51
- Manganese(III) tetrakis(1-methylpyridinium-4-yl)porphyrin 2.124
- Manganese(II) 1,3,5,8-tetramethyl-2,4-diethyl-6,7-di(3-dimethylaminopropyl)porphyrin, dimethanesulfonate 2.51
- Manganese(III) 5,10,15,20-tetraphenylporphyrin 2.144
- Manganese(II) texaphyrin, hydroxide 2.222
- Mequitazine 3.141
- Merbromin 1.157
- Mercurochrome 1.157
- Mercury(II) 7,12-diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.182
- Mercury(II) mesoporphyrin IX, dimethyl ester 2.182
- Merocyanine 540 3.32
- Mesodiphenylbenzhanthrene 1.303
- Mesodiphenylbenzhanthrene 1.139
- Mesoporphyrin bound to  $\alpha$ -(4-bromomethylbenzamido)benzyl]poly(styrene-co-divinylbenzene) 3.106
- Mesoporphyrin bound to  $\alpha$ -(4-bromomethyl-3-nitrobenzamido)benzyl]poly(styrene-co-divinylbenzene) 3.105
- Mesoporphyrin bound to poly(styrene-co-divinylbenzene) 3.104
- Mesoporphyrin di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) ester 2.174
- Mesoporphyrin di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) ester bound to poly(styrene-co-divinylbenzene) 3.105
- Mesoporphyrin di[4-(diphenylmethylaminocarbonylphenylmethyl) ester 2.175
- Mesoporphyrin di[4-(diphenylmethylaminocarbonylphenylmethyl) ester bound to poly(styrene-co-divinylbenzene) 3.106
- Mesoporphyrin diester with *N*-benzhydryl-4-bromomethylbenzamide 2.175
- Mesoporphyrin diester with *N*-benzhydryl-4-bromomethyl-3-nitrobenzamide 2.174
- Mesoporphyrin [4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) methyl ester 2.186
- Mesoporphyrin [4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) monoester 2.187
- Mesoporphyrin IX-*d*<sub>2</sub>, dimethyl ester 2.178
- Mesoporphyrin IX, diethyl ester 2.176
- Mesoporphyrin IX, dimethyl ester 2.177
- Mesoporphyrin IX dimethanesulfonate-6,7-di(methylaminopropyl) derivative 2.49
- Mesoporphyrin methyl ester with *N*-benzhydryl-4-bromomethyl-3-nitrobenzamide 2.186
- Mesoporphyrin monoester with *N*-benzhydryl-4-bromomethyl-3-nitrobenzamide 2.187
- Mesoverdin methyl ester 2.227

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| Methanaminium, <i>N</i> -[4-[(4-(dimethylamino)phenyl)[4-(phenylamino)-1-naphthalenyl]methylene]-2,5-cyclohexadien-1-ylidene]- <i>N</i> -methyl-, chloride | 3.107 |
| Methaniminium, <i>N</i> -[4-[(4-(dimethylamino)phenyl)phenylmethylene]-2,5-cyclohexadiene-1-ylidene]- <i>N</i> -methyl-                                    | 3.103 |
| Methoxsalen  | 1.260 |
| 3'-Methoxyacetophenone   | 1.4   |
| 4'-Methoxyacetophenone   | 1.5   |
| 9-Methoxyfuro[3,2- <i>g</i> ][1]benzopyran-7-one   | 1.260 |
| 5-Methoxy-4-[2-(methylsulfonyl)-4-nitrophenyl]azo-1-naphthoxide ion  | 3.121 |
| 6-Methoxy-3-methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1-(4-ido-1,3,5-heptatrienyl)benzothiazolium, tetrafluoroborate                                    | 3.29  |
| 2-Methoxyphenothiazine   | 1.242 |
| 4'-Methoxypivalothiophenone  | 1.250 |
| 5-Methoxysoralen   | 1.258 |
| 8-Methoxysoralen   | 1.260 |
| 5-Methoxysoralen-DNA complex   | 1.259 |
| Methyl acetal of oxidized octaethylpurpurin ethyl ester  | 2.7   |
| 2-Methylacetophenone biradical   | 1.6   |
| 10-Methyl-9-acridinethione   | 1.8   |
| 4-Methylangelicin  | 1.203 |
| 4'-Methylangelicin   | 1.206 |
| 5-Methylangelicin  | 1.204 |
| 5'-Methylangelicin   | 1.205 |
| 9-Methylanthracene   | 1.26  |
| 1,1'-Methylenebis(6-naphthalenesulfonate ion)  | 3.119 |
| Methylene Blue cation  | 1.245 |
| 1-(2-Methylenephenoxy)-1-hydroxyethyl  | 1.6   |
| 1-Methylindole   | 1.217 |
| 1-Methylnaphthalene  | 1.223 |
| Methyl 2-naphthyl ketone   | 1.1   |
| 1-(4-Methyl-2-nitrophenylazo)-2-naphthol   | 3.130 |
| <i>meso</i> -Methyloctaethylporphinatozinc(II)   | 2.87  |
| 21-Methyl-2,3,7,8,12,13,17,18-octaethylporphine- <i>d</i> <sub>2</sub>   | 2.57  |
| <i>meso</i> -Methyloctaethylporphine   | 2.85  |
| <i>meso</i> -Methyloctaethylporphine- <i>d</i> <sub>2</sub>  | 2.56  |
| <i>N</i> -Methyloctaethylporphyrin   | 2.88  |
| <i>N</i> -Methyloctaethylporphyrin- <i>d</i> <sub>2</sub>  | 2.57  |
| 2-Methyl-4-oxo-1,2-benzothiazine 1,1-dioxide   | 3.24  |
| 10-Methylphenothiazine   | 1.243 |
| <i>N</i> -Methylphenothiazine  | 1.243 |
| 3-Methyl-6-(phenylamino)dibenz[ <i>f,i,j</i> ]isoquinoline-2,7-dione   | 3.63  |
| 1-(4-Methylphenylazo)-3-(phenylaminocarbonyl)-2-naphthol   | 3.115 |
| 1-(4-Methylphenylazo)-1-(phenylaminocarbonyl)-2-propanone  | 3.61  |
| 3-(4-Methylphenyl)-4-phenylsydnone   | 1.282 |
| 3-(4-Methylphenyl)sydnone  | 1.281 |
| Methyl propyl ketone   | 1.230 |
| <i>O</i> -Methyl Rose Bengal methyl ester  | 1.186 |
| 2-Methyl- $\alpha$ -terthienyl   | 1.289 |
| <i>N</i> -Methylthioacridone   | 1.8   |
| ( <i>E,E,E</i> )-5-Methyl-7-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6-heptatrienal   | 1.214 |
| 3-Methyl-2-[7-(1,3,3-trimethyl-2-indolylidene)-1,3,5-heptatrienyl]benzothiazolium, iodide  | 3.30  |
| Michler's ketone   | 1.89  |
| Monohydroxyethyl vinyl deuteroporphyrin  | 2.195 |
| Nalidixic acid   | 3.133 |
| Nalidixic acid, anion  | 3.134 |
| Naphthalocyanine, bis( <i>tri-n</i> -hexyloxysiloxy)silicon  | 2.11  |
| Naphthacene  | 1.291 |
| 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-                                 | 3.108 |
| 5,12-Naphthacenedione, 8-acetyl-10[(3-amino-2,3,6-trideoxy-hexopyranosyloxy)-tetrahydro-6,8,11-trihydroxy-1-methoxy-                                       | 3.109 |
| 5,12-Naphthacenedione, 8-acetyl-7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-1-methoxy- ( <i>S-cis</i> )   | 3.110 |
| 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy- $\alpha$ -L-lyxo-hexopyranosyloxy)-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-  | 3.111 |
| 12-Naphthaceneone, 8-acetyl-10[(3-amino-2,3,6-trideoxyhexopyranosyloxy)-tetrahydro-6,7,11-trihydroxy-5-imino-1-methoxy-                                    | 3.112 |
| Naphthalene  | 1.220 |
| Naphthalene, 2-acetyl-   | 1.1   |
| Naphthalene, 1-bromo-  | 1.222 |
| Naphthalene, 1-methyl-   | 1.223 |
| 2-Naphthaleneacetic acid, 6-methoxy- $\alpha$ -methyl-   | 3.113 |
| 2-Naphthalenecarboxamide, 4-[(4-aminocarbonyl)phenyl]azo]-3-hydroxy- <i>N</i> -(2-methoxyphenyl)-  | 3.114 |
| 2-Naphthalenecarboxamide, 3-hydroxy-4-[(4-methylphenyl)azo]- <i>N</i> -phenyl-   | 3.115 |
| 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-(phenylamino)-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[(2-sulfophenyl)azo]-, trisodium salt                   | 3.116 |
| Naphthalene excimer  | 1.221 |
| 6-Naphthalenesulfonate ion, 1,1'-methylenabis-   | 3.119 |
| 1-Naphthalenesulfonic acid, 3-[[4-chloro-6-(4-methyl-2-sulfophenyl)amino]-1,3,5-triazen-2-yl]amino-3-(5-sulfophenyl)]azo]-, trisodium salt                 | 3.117 |
| 1-Naphthalenesulfonic acid, 5-hydroxy-6-[[2-methoxy-5-[(2-sulfoxyethyl)sulfonyl]phenyl]azo]-, disodium salt  | 3.118 |
| 2-Naphthalenethione, 1,1-dimethyl-   | 1.224 |
| 2-Naphthalenethione, 1,1,3-trimethyl-  | 1.225 |

- Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)- 2.8
- Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)-, chloroaluminum(III) 2.9
- Naphthalocyanine, 2,11,20,29-tetrakis(1,1-dimethylethyl)-, copper(II) 2.10
- 1-Naphthol, 5-[[3-(aminosulfonyl)phenyl]sulfonylamino]-4-[2-(methylsulfonyl)-4-nitrophenylazo]-, conjugate base 3.120
- 1-Naphthol, 5-methoxy-4-[2-(methylsulfonyl)-4-nitrophenyl]azo-, conjugate base 3.121
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, aluminum(III) salt 3.122
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, chromium(III) salt 3.123
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, cobalt(II) salt 3.124
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, cobalt(III) salt 3.125
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, copper(II) salt 3.126
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, iron(III) salt 3.127
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, nickel(II) salt 3.128
- 2-Naphthol, 1-(2-hydroxyphenylazo)-, zinc(II) salt 3.129
- 2-Naphthol, 1-(4-methyl-2-nitrophenylazo)- 3.130
- 2-Naphthol, 1-(4-methylphenylazo)-3-(phenylaminocarbonyl)- 3.115
- 2-Naphthol, 1-(4-nitrophenylazo)- 3.131
- Naphtho[1,8-*bc*]thiopyran-3-one, 2-(1-oxonaphtho[2,1-*b*]thiophen-2-ylidene)-, (*E*) 3.132
- (*E*)-2-[2-(2-Naphthyl)ethenyl]anthracene 1.27
- (*Z*)-2-[2-(2-Naphthyl)ethenyl]anthracene 1.28
- 2-(1-Naphthyl)thiophene 1.297
- 2-(2-Naphthyl)thiophene 1.298
- 1,8-Naphthyridine-3-carboxylic acid, 1,4-dihydro-1-ethyl-7-methyl-4-oxo- 3.133
- 1,8-Naphthyridine-3-carboxylic acid, 1,4-dihydro-1-ethyl-7-methyl-4-oxo-, anion 3.134
- Naproxen 3.113
- Neoalloocimene 1.228
- Nickel(II) bis[2-(4,5-diphenylimidazol-2-yl)azo-5-methylbenzoate] 3.90
- Nickel(II) 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid 2.160
- Nickel(II) 2-(4,5-diphenylimidazol-2-yl)azo-4-nitrophenolate 3.94
- Nickel(II) hematoporphyrin IX 2.160
- Nickel(II) 1-(2-hydroxyphenylazo)-2-naphtholate 3.128
- Nickel(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.125
- Nickel(II) 5,10,15,20-tetraphenylporphyrin 2.145
- 5-Nitroetioporphyrin I 2.99
- 1-(4-Nitrophenylazo)-2-naphthol 3.131
- Norharman 1.226
- 1,4,8,11,15,18,22,25-Octabutoxyphthalocyanatozinc(II) 2.26
- Octaethylchlorin 2.84
- Octaethylchlorin-*d*<sub>2</sub> 2.55
- Octaethylidihydropurpurin ethyl ester 2.14
- 2,3,7,8,12,13,17,18-Octaethyl-5-methylporphinatozinc(II) 2.87
- 2,3,7,8,12,13,17,18-Octaethyl 5 methylporphine 2.85
- 2,3,7,8,12,13,17,18-Octaethyl-5-methylporphine-*d*<sub>2</sub> 2.56
- 2,3,7,8,12,13,17,18-Octaethyl-21-methylporphine 2.88
- 2,3,7,8,12,13,17,18-Octaethyl-5-phenylporphine 2.89
- 2,3,7,8,12,13,17,18-Octaethyl-5-phenylporphine-*d*<sub>2</sub> 2.58
- 2,3,7,8,12,13,17,18-Octaethylporphinatocadmium(II) 2.74
- 2,3,7,8,12,13,17,18-Octaethylporphinatocopper(II) 2.75
- Octaethylporphinatoindium(II) 2.77
- 2,3,7,8,12,13,17,18-Octaethylporphinatolead(II) 2.76
- Octaethylporphinatooxotitanium(IV) 2.78
- Octaethylporphinatooxovanadium(IV) 2.79
- 2,3,7,8,12,13,17,18-Octaethylporphinatopalladium(II) 2.80
- Octaethylporphinatoscandium(III) 2.81
- 2,3,7,8,12,13,17,18-Octaethylporphinatotin(IV) dichloride 2.82
- 2,3,7,8,12,13,17,18-Octaethylporphinatozinc(II) 2.83
- 2,3,7,8,12,13,17,18-Octaethylporphine 2.73
- 2,3,7,8,12,13,17,18-Octaethyl-5-porphinepropenoic acid ethyl ester 2.201
- Octaethylporphyrin 2.73
- Octaethylporphyrin-*d*<sub>2</sub> 2.54
- Octaethylpurpurin ethyl ester 2.16
- 2,3,7,8,12,13,17,18-Octamethyl-5,10,15,20-tetraphenylporphine 2.90
- Octamethyltetraphenylporphyrin 2.90
- Octamethyltetraphenylporphyrin-*d*<sub>2</sub> 2.59
- 1,1',3,3',3',5,5'-Octamethyltricarbocyanine, iodide 3.204
- 1,3,5,7-Octatetraene, 1,8-diphenyl- 1.227
- 2,4,6-Octatriene, 2,6-dimethyl- 1.228
- Oraflex 3.31
- Osmium(II) (4,7-diphenyl-1,10-phenanthroline)bis(1,10-phenanthroline)- 1.141
- 2,2'-Oxatricarbocyanine, 3,3'-diethyl-, iodide 3.135
- (*E*)-2-(1-Oxonaphtho[2,1-*b*]thiophen-2-ylidene)naphtho[1,8-*bc*]thiopyran-3-one 3.132
- Oxovanadyl(IV) sulfophthalocyanine 2.37
- Palladium(II) bis(azido)(4,7-diphenyl-1,10-phenanthroline) 3.46
- Palladium(II) bis(azido)(1,10-phenanthroline) 3.48
- Palladium(II) 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid 2.161
- Palladium(II) 4-*tert*-butylcatechol(1,10-phenanthroline) 3.50

- Palladium(II) catechol(1,10-phenanthroline) 3.53  
 Palladium(II) 3,4-dimercaptotoluene(1,10-phenanthroline) 3.74  
 Palladium(II) hematoporphyrin IX 2.161  
 Palladium(II) mesoporphyrin IX, dimethyl ester 2.183  
 Palladium(II) octaethylporphyrin 2.80  
 Palladium(II) 1,10-phenanthroline(thiosalicylate) 3.139  
 Palladium(II) protoporphyrin dimethyl ester 2.171  
 Palladium(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.126  
 Palladium(II) tetrakis(4-N-methylpyridyl)porphyrin 2.126  
 Palladium(II) tetrakis(4-sulfonatophenyl)porphyrin 2.130  
 Para Red 3.131  
 1,3,3,7,7-Pentamethylbicyclo[2.2.1]heptane-2-thione 1.112  
 3-Pantanethione, 2,2,4,4-tetramethyl- 1.229  
 2-Pantanone 1.230  
 3-Pantanone 1.231  
 3-Pantanone, 2,4-dimethyl- 1.232  
 Perinaphthenone 1.235  
 (E)-Perinaphthothioindigo 3.132  
*trans*-Perinaphthothioindigo 3.132  
 Perylene 1.233  
 Perylo[1,12-def]-1,3-dioxepin-5,11-dione, 6,12-dihydroxy-8,9-bis(2-hydroxypropyl)-7,10-dimethoxy- 1.234  
 Phenalen-1-one 1.235  
 Phenalen-1-one, 6-amino- 1.236  
 Phenanthrene 1.237  
 (1,10-Phenanthroline)bis(thiocyanato)platinum(II) 3.136  
 1,10-Phenanthroline(2,3-naphthalenediolato)platinum(II) 3.137  
 1,10-Phenanthroline(2,3-naphthalenediolato)platinum(II) 3.138  
 1,10-Phenanthroline(thiosalicylato)palladium(II) 3.139  
 1,10-Phenanthrolinetris(1-thienyl-4,4,4-trifluoro-1,3-butanedionato)europium(III) 3.140  
 Phenanthro[1,10,9,8-*opqra*]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- 1.238  
 Phenazine 1.239  
 Phenazinium, 3,7-diamino-2,8-dimethyl-5-phenyl- 3.183  
 Phenol, 2-chloro-4-hydroxy- 1.82  
 Phenol, 4-chloro-3-hydroxy- 1.80  
 Phenol, 2,2',2'',2'''-porphine-5,10,15,20-tetrayl)tetrakis-2.111  
 Phenol, 3,3',3'',3'''-porphine-5,10,15,20-tetrayl)tetrakis-2.112  
 Phenol, 4,4',4'',4'''-porphine-5,10,15,20-tetrayl)tetrakis-2.113  
 Phenothiazine 1.240  
 Phenothiazine, 2-acetyl- 1.241  
 Phenothiazine, 10-(1-azabicyclo[2.2.2]oct-3-ylmethyl)-3.141  
 Phenothiazine, 2-chloro-10-dimethylaminopropyl- 3.142  
 Phenothiazine, 2-methoxy- 1.242  
 Phenothiazine, 10-methyl- 1.243  
 Phenothiazine, 2-(trifluoromethyl)- 1.244  
 Phenothiazine-10-propanamine, 2-chloro-*N,N*-dimethyl-3.142  
 Phenothiazinium, 3,7-bis(dimethylamino)- 1.245  
 Phenothiazinium, 3,7-diamino- 1.246  
 12-(10'-Phenothiazinyl)dodecyl-1-sulfonate ion 3.143  
 9-Phenylanthracene 1.29  
 1-(Phenylazo)-1-(phenylaminocarbonyl)-2-propanone 3.62  
 2-Phenyl-1-benzopyran-4-one 1.98  
 2-Phenylchromone 1.98  
 2,2'-(1,3-Phenylene)bisthiophene 1.299  
 2,2'-(1,4-Phenylene)bisthiophene 1.300  
 (E)-2-(2-Phenylethenyl)anthracene 1.31  
 (Z)-2-(2-Phenylethenyl)anthracene 1.30  
 1-Phenyl-1,2-propanedione 1.251  
 9-(Phenylsulfonyl)fluorene anion 1.152  
 3-Phenylsydnone 1.283  
 4-Phenylthiobenzophenone 1.294  
 Pheophorbide *a* 2.22  
 Pheophytin *a* 2.12  
 Pheophytin *b* 2.13  
 Phloxine B dianion 1.166  
 20-Phorbinecarboxylic acid, 3,4-didehydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester 2.14  
 20-Phorbinecarboxylic acid, 3,4-didehydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester, dichlorotin(IV) 2.15  
 20-Phorbinecarboxylic acid, 3,4,20,21-tetradehydro-3,4,8,9,13,14,18,19-octaethyl-18,19-dihydro-, ethyl ester 2.16  
 20-Phorbinecarboxylic acid, 3,4,20,21-tetradehydro-4,9,14,19-tetraethyl-18,19-dihydro-3,8,13,18-tetramethyl-, ethyl ester, zinc(II) 2.17  
 3-Phorbinepropanoic acid, 9-acetyl-14-ethyl-13,14-dihydro-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester 2.18  
 3-Phorbinepropanoic acid, 9-acetyl-14-ethylidenc-13,14-dihydro-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester 2.19  
 3-Phorbinepropanoic acid, 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, magnesium(II) 2.20  
 3-Phorbinepropanoic acid, 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-, 3,7,11,15-tetramethyl-2-hexadecenyl ester 2.21  
 3-Phorbinepropanoic acid, 9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,6,13,18-tetramethyl-20-oxo-2.22

- 3-Phorbinepropanoic acid, [3,7,11,15-tetramethyl-2-hexadecenyl 3,4-didehydro-9-ethenyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-phorbinepropanoatomagnesium 2.23
- Photofrin II 3.144
- Photoprotoporphyrin IX dimethyl ester 2.196
- Phthalocyaninatobis(pyridine)zinc(II) 2.25
- Phthalocyaninatomagnesium(II) 2.24
- Phthalocyanine, magnesium(II) 2.24
- Phthalocyanine, 1,4,8,11,15,18,22,25-octabutoxy-, zinc(II) 2.26
- Phthalocyanine, sulfo- 2.27
- Phthalocyanine, sulfo-, chloroaluminum(III) 2.29
- Phthalocyanine, sulfo-, chlorogallium(III) 2.36
- Phthalocyanine, sulfo-, cobalt(II) 2.32
- Phthalocyanine, sulfo-, copper(II) 2.33
- Phthalocyanine, sulfo-, iron(II) 2.34
- Phthalocyanine, sulfo-, oxovanadium(IV) 2.37
- Phthalocyanine, sulfo-, zinc(II) 2.39
- Phthalocyanine, tetracarboxy-, copper(II) 2.40
- Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)- 2.41
- Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)-, chloroaluminum(III) 2.42
- Phthalocyanine, 2,9,16,23-tetrakis(1,1-dimethylethyl)-, copper(II) 2.43
- Phthalocyanine, [2,9,16,23-tetrakis(1,1-dimethylethyl)]-, magnesium(II) 2.44
- Phthalocyanine, tetrakis[methylenethio[(dimethylamino)methylidyne]]tetrakis[N-methylmethanaminiumato]-, copper(II), tetrachloride 2.45
- Phthalocyanine, tetrasulfo-, chlorogallium(III) 2.35
- Phthalocyanine, trisulfo-, chloroaluminum(III) 2.28
- Phthalocyanine, trisulfo-, zinc(II) 2.38
- Phthalocyanine, zinc(II), bis(pyridine) 2.25
- Phycocyanobilin dimethyl ester 3.33
- Pigment Red 1 3.131
- Pigment Red 3 3.130
- Piroxicam 3.23
- Pivalothiophenone 1.247
- Pivalothiophenone, 4'-chloro- 1.248
- Pivalothiophenone, 4'-fluoro- 1.249
- Pivalothiophenone, 4'-methoxy- 1.250
- Platinum(II) bis(azido)(2,2'-biquinoline) 3.44
- Platinum(II) bis(azido)(4,7-diphenyl-1,10-phenanthroline) 3.47
- Platinum(II) bis(azido)(1,10-phenanthroline) 3.49
- Platinum(II) 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid 2.162
- Platinum(II) catechol(1,10-phenanthroline) 3.54
- Platinum(II) dibromo(1,10-phenanthroline) 3.68
- Platinum(II) dicyano(1,10-phenanthroline) 3.70
- Platinum(II) diiodo(1,10-phenanthroline) 3.73
- Platinum(II) hematoporphyrin IX 2.162
- Platinum(II) (1,10-phenanthroline)bis(thiocyanate) 3.136
- Polycycline 3.108
- Poly(sodium styrenesulfonate-co-2-vinylnaphthalene) 3.145
- Porphine 2.46
- Porphine-21,23-*d*<sub>2</sub> 2.47
- Porphine, 5-amino-2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- 2.48
- Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate 2.49
- Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, cobalt(II) 2.50
- Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, manganese(II) 2.51
- Porphine, 2,18-bis[3-(dimethylammonio)propyl]-7,12-diethyl-3,8,13,17-tetramethyl-, dimethanesulfonate, zinc(II) 2.52
- Porphine, 21,23-dideutero-2,3-dihydro-5,10,15,20-tetraphenyl- 2.53
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-2.54
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-2,3-dihydro- 2.55
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-5-methyl- 2.56
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-21-methyl- 2.57
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl-5-phenyl- 2.58
- Porphine, 21,23-dideutero-2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenyl- 2.59
- Porphine, 21,23-dideutero-2,3,12,13-tetraethyl- 2.60
- Porphine, 21,23-dideutero-2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- 2.61
- Porphine, 21,23-dideutero-5,10,15,20-tetrakis(2-chlorophenyl)- 2.62
- Porphine, 21,23-dideutero-5,10,15,20-tetrakis(3-chlorophenyl)- 2.63
- Porphine, 21,23-dideutero-5,10,15,20-tetrakis(4-chlorophenyl)- 2.64
- Porphine, 21,23-dideutero-5,10,15,20-tetraphenyl- 2.65
- Porphine, 21,23-dideutero-5,10,15,20-tetrapropyl- 2.66
- Porphine, 13,17-diethyl-3,7,8,12,18-pentamethyl-2,20-cyclo(3-oxo-2-propenyl)-, zinc(II) 2.226
- Porphine, 2,3-dihydro-5,10,15,20-tetraphenyl- 2.67
- Porphine, ethanediylibis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-2.68
- Porphine, ethanediylibis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-2.68
- Porphine, ethanediylibis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-2.68

- Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, copper(II) 2.69
- Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octaethyl-, copper(II)zinc(II) 2.70
- Porphine, ethanediylbis[5,5'-(2,3,7,8,12,13,17,18-octapropyl-, biscopper(II) 2.72
- Porphine, 2,3,7,8,12,13,17,18-octaethyl- 2.73
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-, cadmium(II) 2.74
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-, copper(II) 2.75
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-, dichlorotin(IV) 2.82
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-, lead(II) 2.76
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-, palladium(II) 2.80
- Porphine, octaethyl-, indium(II) 2.77
- Porphine, octaethyl-, oxotitanium(IV) 2.78
- Porphine, octaethyl-, oxovanadium(IV) 2.79
- Porphine, octaethyl-, scandium(III) 2.81
- Porphine, octaethyl-, zinc(II) 2.83
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-2,3-dihydro- 2.84
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl- 2.85
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl-, copper(II) 2.86
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-methyl-, zinc(II) 2.87
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-21-methyl- 2.88
- Porphine, 2,3,7,8,12,13,17,18-octaethyl-5-phenyl- 2.89
- Porphine, 2,3,7,8,12,13,17,18-octamethyl-5,10,15,20-tetraphenyl- 2.90
- Porphine, 2,3,7,8-tetraethyl- 2.91
- Porphine, 2,3,12,13-tetraethyl- 2.92
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl- 2.93
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-, zinc(II) 2.94
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10-dinitro- 2.95
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10-dinitro-, zinc(II) 2.96
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,15-dinitro- 2.97
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,15-dinitro-, zinc(II) 2.98
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5-nitro- 2.99
- Porphine, 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10,15-trinitro- 2.100
- Porphine, 7,8,17,18-tetrahydro-5,10,15,20-tetraphenyl-, (E) 2.101
- Porphine, 5,10,15,20-tetrakis(4-bromophenyl)- 2.102
- Porphine, tetrakis(4-carboxyphenyl)- 2.103
- Porphine, 5,10,15,20-tetrakis(4-carboxyphenyl)- 2.103
- Porphine, tetrakis(4-chlorophenyl)- 2.106
- Porphine, 5,10,15,20-tetrakis(2-chlorophenyl)- 2.104
- Porphine, 5,10,15,20-tetrakis(3-chlorophenyl)- 2.105
- Porphine, 5,10,15,20-tetrakis(4-chlorophenyl)- 2.106
- Porphine, 5,10,15,20-tetrakis(2,6-dichloro-3-sulfonatophenyl)-, zinc(II) 2.107
- Porphine, tetrakis(2-fluorophenyl)-, zinc(II) 2.109
- Porphine, 5,10,15,20-tetrakis(2-fluorophenyl)- 2.108
- Porphine, 5,10,15,20-tetrakis(4-fluorophenyl)- 2.110
- Porphine, 5,10,15,20-tetrakis(2-hydroxyphenyl)- 2.111
- Porphine, 5,10,15,20-tetrakis(3-hydroxyphenyl)- 2.112
- Porphine, 5,10,15,20-tetrakis(4-hydroxyphenyl)- 2.113
- Porphine, 5,10,15,20-tetrakis(4-iodophenyl)- 2.114
- Porphine, tetrakis(1-methylpyridinium-2-yl)- 2.115
- Porphine, tetrakis(1-methylpyridinium-3-yl)- 2.116
- Porphine, tetrakis(1-methylpyridinium-4-yl)- 2.117
- Porphine, tetrakis(1-methylpyridinium-4-yl)-, zinc(II) 2.128
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, cadmium(II) ion 2.118
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, cobalt(II) 2.119
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, copper(II) 2.120
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, iron(II) ion 2.121
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, lutetium(III) 2.122
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, magnesium(II) 2.123
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, manganese(III) ion 2.124
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, nickel(II) 2.125
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, palladium(II) ion 2.126
- Porphine, 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)-, tin(IV) ion 2.127
- Porphine, tetrakis(4-sulfonatophenyl)- 2.129
- Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)- 2.129
- Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, dichlorotin(IV) 2.131
- Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, palladium(II) 2.130
- Porphine, 5,10,15,20-tetrakis(4-sulfonatophenyl)-, zinc(II) 2.133
- Porphine, 5,10,15,20-tetrakis(4-trimethylammoniophenyl)- 2.134
- Porphine, 3,7,12,18-tetramethyl-2,8-diethyl- 2.135
- Porphine, 5,10,15,20-tetraphenyl- 2.136
- Porphine, 5,10,15,20-tetraphenyl-, chloroaluminum(III) 2.138
- Porphine, 5,10,15,20-tetraphenyl-, cobalt(II) 2.139
- Porphine, 5,10,15,20-tetraphenyl-, copper(II) 2.140
- Porphine, 5,10,15,20-tetraphenyl-, dichlorotin(IV) 2.141

- Porphine*, 5,10,15,20-tetraphenyl-, gallium(II) 2.142  
*Porphine*, 5,10,15,20-tetraphenyl-, iron(III) 2.143  
*Porphine*, 5,10,15,20-tetraphenyl-, manganese(III) 2.144  
*Porphine*, 5,10,15,20-tetraphenyl-, nickel(II) 2.145  
*Porphine*, 5,10,15,20-tetraphenyl-, zinc(II) 2.146  
*Porphine*, tetraphenyl-, cadmium(II) 2.137  
*Porphine*, 5,10,15,20-tetrapropyl- 2.147  
*Porphine*, 5,10,15-tris(4-N-methylpyridyl)-20-[2-[N-(2-[5,10,15-tris(4-N-methylpyridyl)phenyl]-3-phenoxypropyl)-4-carboxybutyl]phenyl]- 2.148  
*Porphine*-5-carboxaldehyde, 21,23-dideutero-2,3,7,8,12,13,17,18-octaethyl- 2.149  
*Porphine*-5-carboxaldehyde, 2,3,7,8,12,13,17,18-octaethyl- 2.150  
*Porphine*-2,20-dicarboxylic acid, 18-(20-carboxyethyl)-12-ethyl-7-ethyl-17,18-dihydro-3,8,13,17-tetramethyl-, cyclic 2,20-anhydride 2.151  
*Porphine*-2,18-dipropanoic acid, 7,12-bis[1-[(2-amino-2-carboxyethyl)thio]ethyl]-3,8,13,17-tetramethyl- 2.152  
*Porphine*-2,18-dipropanoic acid, 7,12-bis[1-[(2-amino-2-carboxyethyl)thio]ethyl]-3,8,13,17-tetramethyl-, zinc(II) 2.153  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl- 2.154  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, cobalt(III) 2.155  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, copper(II) 2.156  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, dimethyl ester 2.158  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, manganese(III) 2.159  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, nickel(II) 2.160  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, palladium(II) 2.161  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-hydroxyethyl)-3,8,13,17-tetramethyl-, platinum(II) 2.162  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(2-hydroxyethyl)-3,8,13,17-tetramethyl- 2.163  
*Porphine*-2,18-dipropanoic acid, 7,12-bis(1-methoxyethyl)-3,7,12,17-tetramethyl-, dianion 2.164  
*Porphine*-2,18-dipropanoic acid, 21,23-dideutero-7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester 2.167  
*Porphine*-2,18-dipropanoic acid, 21,23-dideutero-7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester 2.178  
*Porphine*-2,18-dipropanoic acid, 21,23-dideutero-3,7,12,17-tetramethyl-, dimethyl ester 2.199  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl- 2.165  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dichlorotin(IV) 2.172  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester 2.166  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, magnesium(II) 2.168  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, palladium(II) 2.171  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, dimethyl ester, zinc(II) 2.169  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, magnesium(II) 2.170  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, zinc(II) 2.173  
*Porphine*-2,18-dipropanoic acid, 7,12-diethenyl-3,8,13,17-tetramethyl-, di[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl)ester] 2.174  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, di[4-(diphenylmethylaminocarbonylphenylmethyl)ester] 2.175  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, diethyl ester 2.176  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester 2.177  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, cadmium(II) 2.179  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, copper(II) 2.180  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, magnesium(II) 2.181  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, mercury(II) 2.182  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, oxovanadium(IV) 2.184  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, palladium(II) 2.183  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, dimethyl ester, zinc(II) 2.185  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, [4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl) methyl ester] 2.186  
*Porphine*-2,18-dipropanoic acid, 7,12-diethyl-3,8,13,17-tetramethyl-, mono[4-(diphenylmethylaminocarbonyl-2-nitrophenylmethyl)ester] 2.187  
*Porphine*-2,18-dipropanoic acid, 7,12-diformyl-3,8,13,17-tetramethyl-, dimethyl ester 2.188  
*Porphine*-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-ethyl-7,8-dihydro-3,7,12,17-tetramethyl-, dimethyl ester, (Z) 2.189  
*Porphine*-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-ethylidene-7,8-dihydro-3,7,12,17-tetramethyl-, dimethyl ester, (Z) 2.190  
*Porphine*-2,18-dipropanoic acid, 7-(2-(dimethylamino)-2-oxoethyl)-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl-, dimethyl ester, (Z) 2.191

- Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, tin(IV), (Z) 2.192
- Porphine-2,18-dipropanoic acid, 7-[2-(dimethylamino)-2-oxoethyl]-8-heptyl-7,8-dihydro-3,7,12,17-tetramethyl, dimethyl ester, zinc(II), (Z) 2.193
- Porphine-2,18-dipropanoic acid, 7(12)-ethenyl-12(7)-formyl, dimethyl ester 2.194
- Porphine-2,18-dipropanoic acid, 7-ethenyl-12-(1-hydroxyethyl)-3,8,13,17-tetramethyl- 2.195
- Porphine-2,18-dipropanoic acid, 12(7)-ethenyl-8(13)-hydroxy-3,8,13,17-tetramethyl-7(12)-(oxoethylidene)-, dimethyl ester 2.196
- Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl- 2.197
- Porphine-2,18-dipropanoic acid, 3,7,12,17-tetramethyl-, dimethyl ester 2.198
- Porphine-2-propanoic acid, 18-carboxy-20-(carboxymethyl)-8-ethenyl-13-ethyl-2,3-dihydro-3,7,12,17-tetramethyl- 2.200
- Porphine-18-propanoic acid, 8,13-diethyl-3,7,12,17-tetramethyl-2,20-cyclo(3-oxo-2-propenyl)- 2.227
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- 5,10,15,20-Tetraphenylporphinato(chloro)aluminum(III) ion **2.138**
- 5,10,15,20-Tetraphenylporphinatocobalt(II) **2.139**
- 5,10,15,20-Tetraphenylporphinatocupper(II) **2.140**
- 5,10,15,20-Tetraphenylporphinatogallium(II) **2.142**
- 5,10,15,20-Tetraphenylporphinatonickel(II) **2.145**
- 5,10,15,20-Tetraphenylporphinatozinc(II) **2.146**
- 5,10,15,20-Tetraphenylporphine **2.136**
- 5,10,15,20-Tetraphenylporphine-*d*<sub>2</sub> **2.65**
- meso*-Tetraphenylporphine **2.136**
- 5,6,11,12-Tetraphenyltetracene **1.278**
- Tetraphenyltetrahydroporphine **2.101**
- 5,10,15,20-Tetrapropylporphine **2.147**
- 5,10,15,20-Tetrapropylporphine-*d*<sub>2</sub> **2.66**
- 2,7,12,17-Tetrapropylporphycene **2.212**
- 2,7,12,17-Tetrapropyl-21,22,23,24-tetraazapentacyclo[16.2.1<sup>2,5</sup>.1<sup>8,11</sup>.1<sup>12,15</sup>]tetracosa-1,3,5,7,9,11(23),12,14,16,18(21),19-undecaene **2.212**
- Tetra(4-*N,N,N*-trimethylanilinium)porphine **2.134**
- 2,2'-Thiatricarbocyanine, 3,3'-diethyl-, iodide **3.194**
- Thiobenzophenone, 4,4'-dimethoxy- **1.293**
- Thiobenzophenone, 4-phenyl- **1.294**
- Thiocamphenilone **1.111**
- Thiocamphor **1.114**
- Thiocoumarin **1.295**
- Thiofenchone **1.113**
- Thioindigo Black **3.102**
- Thioindigo Red Brown G **3.132**
- Thionine cation **1.246**
- ThionorcAMPHOR **1.110**
- Thiophene, 2,5-diphenyl- **1.296**
- Thiophene, 2-(1-naphthalenyl)- **1.297**
- Thiophene, 2-(2-naphthalenyl)- **1.298**
- Thiophene, 2,2'-(1,3 phenylene)bis **1.299**
- Thiophene, 2,2'-(1,4-phenylene)bis- **1.300**
- Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)selenopyran-4-ylidene]-3-propenyl]- **3.195**
- Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)telluropyran-4-ylidene]-3-propenyl]- **3.196**
- Thiopyrylium, 2,6-bis(1,1-dimethylethyl)-4-[1-[2,6-bis(1,1-dimethylethyl)thiopyran-4-ylidene]-3-propenyl]- **3.197**
- 4-Thiouridine **1.301**
- Tin(IV) dichloro[octaethylidihydropurpurin ethyl ester] **2.15**
- Tin(IV) (dichloro)5,10,15,20-tetraphenylporphyrin **2.141**
- Tin(IV) octaethylporphyrin dichloride **2.82**
- Tin(IV) tetrakis(1-methylpyridinium-4-yl)porphyrin **2.127**
- Titanium(IV) (oxo)octaethylporphyrin **2.78**
- Toluidine Red **3.130**
- 1,4,7-Triazacyclonanonetri(isothiocyanato)chromium(III) **1.302**
- Tribenzo[*a,f,j*]perylene, 9,18-diphenyl- **1.303**
- Tribromofluorescein dianion **1.191**
- Tricarbocyanine, 5,5'-dichloro-1,1',3,3,3',3'-hexamethyl-, iodide **3.198**
- Tricarbocyanine, 5,5'-difluoro-1,1',3,3,3',3'-hexamethyl-, iodide **3.199**
- Tricarbocyanine, 5,5'-dimethoxy-1,1',3,3,3',3'-hexamethyl-, iodide **3.200**
- Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, fluoride **3.201**
- Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, iodide **3.202**
- Tricarbocyanine, 1,1',3,3,3',3'-hexamethyl-, perchlorate **3.203**
- Tricarbocyanine, 1,1',3,3,3',3',5,5'-octamethyl-, iodide **3.204**
- 2-Triflumethylphenothiazine **1.244**
- 4-(Trifluoromethyl)benzophenone **1.92**
- 2-(Trifluoromethyl)phenothiazine **1.244**
- 2,4,5-Triiodosuccinylfluorescein bound as copoly(styrene-*p*-vinylbenzyl ester) **3.208**
- 2,4,5-Triiodosuccinylfluorescein dianion **1.314**
- 4,7,4'-Trimethylallopsoralen **1.196**
- 4,7,5'-Trimethylallopsoralen **1.195**
- 6,4,4'-Trimethylangelicin **1.207**
- 1,7,7 Trimethylbicyclo[2.2.1]heptane-2,3-dione **1.109**
- 1,3,3-Trimethylbicyclo[2.2.1]heptane-2-thione **1.113**
- 1,7,7 Trimethylbicyclo[2.2.1]heptane-2-thione **1.114**
- 3,5,5-Trimethyl-2-cyclohexenethione **1.132**
- 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-butene-2-one **1.218**
- 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-(2,2-dimethoxyethyl)-1,3,5-heptatrienyl]-1,1,3-trimethylindolium, tetrafluoroborate **3.99**
- 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-(1-piperidinio)-1,3,5-heptatrienyl]-1,3,3-trimethylindolium, bis(tetrafluoroborate) **3.100**
- 2-[7-(1,3,3-Trimethyl-2-indol-2-ylidene)-1-[4-[3-(1,3,3-trimethyl-2-indolylidene)-2-propenyl]-1,3,5-heptatrienyl]-1,1,3-trimethylindolium, tetrafluoroborate **3.101**
- 1,1,3-Trimethyl-2-naphthalenethione **1.225**
- 4,5',8-Trimethylpsoralen **1.261**
- 5,10,15-Trinitroetioporphyrin I **2.100**
- Trioxsalen **1.261**
- 1,3,5-Triphenylbenzene **1.75**
- Triphenylene **1.304**
- 6,13,20-Triphenyltetrabenzo[*b,g,l,q*]porphinatozinc(II) **2.218**
- Tris(2,2'-bipyridine)iridium(III) ion **1.305**
- Tris(2,2'-bipyridine)ruthenium(II) ion **1.306**
- Tris(2,2'-bipyridine)ruthenium(II) ion bound to Dowex 50W-X1 resin **3.205**

- Tris(1,10-phenanthroline)iridium(III) ion 1.307  
 Tris(1,10-phenanthroline)osmium(II) ion 1.308  
 Tris(1,10-phenanthroline)ruthenium(II) ion 1.309  
 Tris(1,10-phenanthroline)ruthenium(II) ion bound to Dowex 50W-X1 resin 3.206  
 Trypaflavine cation 1.10  
 1,11-Undecanediylibis[3,8,12,17-tetramethyl-2,7,18-tris(2-carboxyethyl)porphine 2.209  
 Uroporphyrin I 2.203  
 Vanadium(IV) (oxo)7,12-diethyl-3,8,13,17-tetramethylporphine-2,18-dipropanoic acid, dimethyl ester 2.184  
 Vanadium(IV) (oxo)mesoporphyrin IX, dimethyl ester 2.184  
 Vanadium(IV) (oxo)octaethylporphyrin 2.79  
 Vat Black B 3.3  
 Vat Brilliant Green G 3.2  
 Vat Brilliant Green Zh 3.2  
 Vat Brilliant Orange KKh 3.64  
 Vat Brilliant Orange RK 3.64  
 Vat Brilliant Violet R 3.4  
 Vat Brown R 3.75  
 Vat Dark Blue BO 3.1  
 Vat Dark Blue O 3.1  
 Vat Golden Yellow GK 3.65  
 Vat Golden Yellow RK 3.66  
 Victoria Blue B 3.107  
 2-Vinylanthracene 1.34  
 Violanthrone 3.1  
 Vitamin A 1.273  
 Vitamin B<sub>2</sub> 1.274  
 Vitamin D<sub>3</sub> 1.310  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-4,5-diiodo-, dianion 1.311  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetrabromo-, dianion 1.312  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetraido-, dianion 1.313  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5,7-tetraido-, dianion, bound as copoly(styrene-p-vinylbenzyl ester) 3.207  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5-triido-, dianion 1.314  
 Xanthen-3-one, 9-(2-carboxyethyl)-6-hydroxy-2,4,5-triido-, dianion, bound as copoly(styrene-p-vinylbenzyl ester) 3.208  
 Xanthen-3-one, 9-(2,3,4,5-tetrachlorophenyl)-6-hydroxy-2,4,5,7-tetraido-, anion 1.315  
 Xanthen-9-one 1.316  
 Xanthone 1.316  
 Xanthotoxin 1.260  
 Xanthylum, 9-(2-carboxyphenyl)-3,6-bis(diethylamino)-3.165  
 Xanthylum, 9-[2-(ethoxycarbonyl)phenyl]-3,6-bis(ethylamino)-2,7-dimethyl- 3.166  
 Ytterbium(II) 5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin 2.132  
 Zinc(II) chlorotexaphyrin chloride 2.224  
 Zinc(II) 5,10-dinitroetioporphyrin I 2.96  
 Zinc(II) 5,15-dinitroetioporphyrin I 2.98  
 Zinc(II) diphenyltetrazenobenzoporphyrin 2.217  
 Zinc(II) etioporphyrin 2.94  
 Zinc(II) etiopurpurin ethyl ester 2.17  
 Zinc(II) 1-(2-hydroxyphenylazo)-2-naphtholate 3.129  
 Zinc(II) mesoporphyrin IX, dimethyl ester 2.185  
 Zinc(II) mesoporphyrin IX dimethanesulfonate-6,7-di(methylaminopropyl) derivative 2.52  
 Zinc methyl pyroverdin 2.226  
 Zinc(II) 1,4,8,11,15,18,22,25-octabutoxyphthalocyanine 2.26  
 Zinc(II) 2,3,7,8,12,13,17,18-octaethylporphyrin 2.87  
 Zinc(II) octaethylporphyrin 2.83  
 Zinc(II) 2,3,7,8,12,13,17,18-octaethylporphyrin 2.83  
 Zinc(II) phthalocyaninebis(pyridine) 2.25  
 Zinc(II) porphyrin c 2.153  
 Zinc(II) protoporphyrin 2.173  
 Zinc(II) protoporphyrin, dimethyl ester 2.169  
 Zinc(II) protoporphyrin IX 2.173  
 Zinc(II) sulfophthalocyanine 2.39  
 Zinc(II) tetrabenzoporphyrin 2.214  
 Zinc(II) 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,10-dinitroporphyrin 2.96  
 Zinc(II) 2,7,12,17-tetraethyl-3,8,13,18-tetramethyl-5,15-dinitroporphyrin 2.98  
 Zinc(II) 2,7,12,17-tetraethyl-3,8,13,18-tetramethylporphyrin 2.94  
 Zinc(II) tetrakis(2,6-dichloro-3-sulfonatophenyl)porphyrin 2.107  
 Zinc(II) tetrakis(2-fluorophenyl)porphyrin 2.109  
 Zinc(II) 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin 2.128  
 Zinc(II) tetrakis(4-N-methylpyridyl)porphyrin 2.128  
 Zinc(II) tetrakis(4-sulfonatophenyl)porphyrin 2.133  
 Zinc(II) 1,3,5,8-tetramethyl-2,4-diethyl-6,7-di-(3-dimethylaminopropyl)porphyrin, dimethanesulfonate 2.52  
 Zinc(II) tetraphenylporphyrin 2.146  
 Zinc(II) texaphyrin chloride 2.225  
 Zinc(II) triphenyltetrazenobenzoporphyrin 2.218  
 Zinc(II) trisulfophthalocyanine 2.38

## 12. Appendix 1. Reverse Energy Transfer and Geminate Reactions

### 12.1. Reverse Energy Transfer

The treatment given in the main article does not consider reverse energy transfer to and from singlet oxygen from the sensitizers. This would only be expected to be important when the energy of the sensitizer triplet is close to that of singlet oxygen. In order to see the effect of reverse energy transfer we treat first Scheme 1 without reverse energy transfer.

#### 12.1.1. Derivation of $\phi_\Delta$ according to Scheme 1, i.e. without energy transfer for self-sensitized photo-oxidation.

Applying the steady-state treatment to  $S_1$ ,  $T_1$  and  $^1O_2^*$  gives

$$\frac{d[S_1]}{dt} = 0 = I_a - (k_{SD} + k_{SQ}^{O_2}[O_2])[S_1],$$

therefore

$$\frac{[S_1]}{I_a} = \frac{1}{(k_{SD} + k_{SQ}^{O_2}[O_2])} = \frac{(1 - P_S^{O_2})}{k_{SD}}. \quad (A.1)$$

$$\begin{aligned} \frac{d[T_1]}{dt} = 0 &= (f_T^{O_2} k_{SQ}^{O_2}[O_2] + k_{isc})[S_1] \\ &- (k_{TD} + k_{TQ}^{O_2}[O_2])[T_1], \end{aligned}$$

therefore

$$\begin{aligned} \frac{[T_1]}{I_a} &= \frac{f_T^{O_2} k_{SQ}^{O_2}[O_2] + k_{isc}}{(k_{SD} + k_{SQ}^{O_2}[O_2])(k_{TD} + k_{TQ}^{O_2}[O_2])} \\ &= \frac{f_T^{O_2} P_S^{O_2} + \phi_T(1 - P_S^{O_2})}{k_{TD} + k_{TQ}^{O_2}[O_2]} \end{aligned} \quad (A.2)$$

and in the presence of a reactive substrate i.e. with  $M = A$  we obtain

$$\begin{aligned} \frac{d[^1O_2^*]}{dt} = 0 &= f_\Delta^S k_{SQ}^{O_2}[O_2][S_1] + f_\Delta^T k_{TQ}^{O_2}[O_2][T_1] \\ &- (k_\Delta + k_A[A])[^1O_2^*]. \end{aligned}$$

Substitution of Eqs. (A.1) and (A.2) gives

$$\frac{[^1O_2^*]}{I_a} = \frac{f_\Delta^S P_S^{O_2} + f_\Delta^T P_T^{O_2} f_T^{O_2} P_S^{O_2} + f_\Delta^T P_T^{O_2} \phi_T(1 - P_S^{O_2})}{(k_\Delta + k_A[A])}. \quad (A.3)$$

The quantum yield of photo-oxidation of  $A$  by singlet oxygen is

$$\phi_{ox} = \frac{k_r^A[A][^1O_2^*]}{I_a} = \frac{k_r^A[A]}{(k_\Delta + k_A[A])} \phi_\Delta \quad (A.4)$$

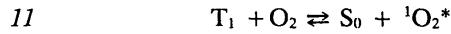
and from (A.3) and (A.4)

$$\phi_\Delta := f_\Delta^S P_S^{O_2} + f_\Delta^T P_T^{O_2} f_T^{O_2} P_S^{O_2} + f_\Delta^T P_T^{O_2} \phi_T(1 - P_S^{O_2}). \quad (A.5)$$

N.B. (A.4) and (A.5) are Eqs. (14) and (1) respectively in the main text.

#### 12.1.2. Derivation of $\phi_\Delta$ in the presence of back energy transfer

Application of the steady-state approximation to  $S_1$ ,  $T_1$  and  $^1O_2^*$  according to Scheme 1, including back energy transfer i.e. step 11 written as



$$\text{where } k_{11} = k_{T\Delta}^O \text{ and } k_{-11} = k_{\Delta T}.$$

Equation (A.1) is unaffected, however now

$$\begin{aligned} \frac{d[T_1]}{dt} = 0 &= (f_T^{O_2} k_{SQ}^{O_2}[O_2] + k_{isc})[S_1] \\ &+ k_{\Delta T}[A][^1O_2^*] - (k_{TD} + k_{TQ}^{O_2}[O_2])[T_1] \end{aligned}$$

and

$$\begin{aligned} \frac{d[^1O_2^*]}{dt} = 0 &= f_\Delta^S k_{SQ}^{O_2}[O_2][S_1] + f_\Delta^T k_{TQ}^{O_2}[O_2][T_1] \\ &- (k_\Delta + k_A[A] + k_{\Delta T}[A])[^1O_2^*]. \end{aligned}$$

If we define

$$\alpha = \frac{k_{\Delta T}[A]}{k_\Delta + k_A[A] + k_{\Delta T}[A]}, \quad (A.6)$$

$$\frac{[T_1]}{I_a} = \frac{f_T^{O_2} P_S^{O_2} + \phi_T(1 - P_S^{O_2}) + f_\Delta^S P_S^{O_2} \alpha}{k_{TD} + k_{TQ}^{O_2}[O_2] - f_\Delta^T k_{TQ}^{O_2}[O_2] \alpha} \quad (A.7)$$

and

$$\frac{[^1O_2^*]}{I_a} = \frac{f_\Delta^S P_S^{O_2} + f_\Delta^T P_T^{O_2} \{f_T^{O_2} P_S^{O_2} + \phi_T(1 - P_S^{O_2})\}}{k_\Delta + k_A[A] + k_{\Delta T}[A](1 - f_\Delta^T P_T^{O_2})}. \quad (A.8)$$

Thus with back transfer

$$\phi_{ox} = \frac{[f_\Delta^S P_S^{O_2} + f_\Delta^T P_T^{O_2} f_T^{O_2} P_S^{O_2} + f_\Delta^T P_T^{O_2} \phi_T(1 - P_S^{O_2})]}{k_\Delta + k_A[A] + k_{\Delta T}[A](1 - f_\Delta^T P_T^{O_2})} k_r^A[A]. \quad (A.9)$$

Equation (A.9) may be considered in two equivalent ways<sup>1</sup>, firstly, where  $\phi_\Delta$  remains unchanged and back transfer increases the physical quenching of singlet oxygen. However, secondly, if reverse energy transfer occurs and one uses Eq. (14) or (A.4) derived without considering it i.e. by putting

$$\phi_{ox} = \frac{\phi_\Delta k_r^A[A]}{k_\Delta + k_A[A]}, \quad (A.10)$$

then the reverse energy transfer would be considered as reducing the quantum yield of singlet oxygen production and thus from Eqs. (A.9) and (A.10)

$$\phi_\Delta^b = \frac{\phi_\Delta (k_\Delta + k_A[A])}{k_\Delta + k_A[A] + k_{\Delta T}[A](1 - f_\Delta^T P_T^{O_2})}, \quad (A.11)$$

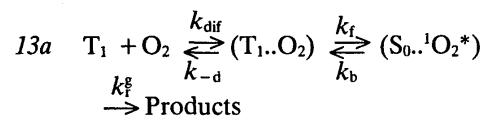
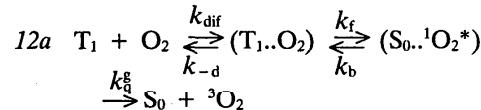
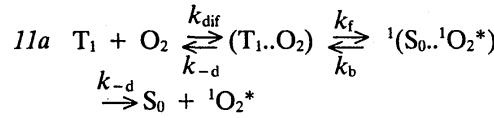
and

$$\phi_{\Delta}^b = \frac{\phi_{\Delta}(1-\alpha)}{1-\alpha f_{\Delta}^b P_1^{O_2}}. \quad (A.12)$$

We recommend that when reverse energy transfer is expected it be taken into account and the quantum yield of singlet oxygen production taken as unchanged as in Eq. (A.9).

## 12.2. Geminate Reaction

Wilson<sup>2</sup> reported that the direct, i.e. self-sensitized, photo-oxidation of DPBF could be inhibited by the addition of TME but that inhibition was never total and a residual rate of self-oxidation remains at high concentration of TME. Stevens *et al.*<sup>3</sup>, Drews *et al.*<sup>4</sup> and Merkel and Kearns<sup>5</sup> have discussed various aspects of this problem which pertain to the question of the reactions of correlated pairs of molecules. Thus for example in the case of self-sensitized photo-oxidation the triplet state of the substrate, A = S, is quenched by O<sub>2</sub>, thus we can write in place of reactions 11, 12, and 13 in Scheme 1

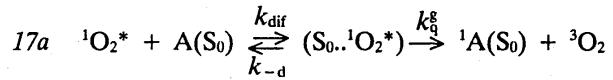
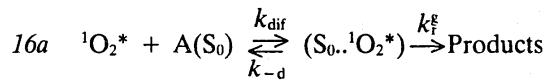


where  $k_q^g$  and  $k_q^h$  are geminate reaction probabilities of the encounter complex ( $S_0..^1O_2^*$ ) i.e. prior to achievement of what may be considered to be a random or homogeneous separation which can be reached with a probability  $k_{-d}$ . Thus  $k_q^g$  and  $k_q^h$  include any orbital or symmetry restrictions and any re-encounters of this correlated pair. When  $k_b$  is very small i.e. when no reverse energy transfer occurs e.g. when  $E_{T_1} \gg E_{\Delta}$  the quantum yield of geminate recombination is

$$\phi_{\text{ox}}^g = \phi_{\Delta} f_{\text{r}}^g = \frac{\phi_{\Delta} k_{\text{r}}^g}{k_{-d} + k_{\text{r}}^g + k_q^g} \quad (A.13)$$

where  $f_{\text{r}}^g$  is the fraction of coordinated pairs which are formed which undergo geminate reaction. Note that  $\phi_{\text{ox}}^g$  is independent of [A] and  $\tau_{\Delta}$  and can be measured from studies of very low values of [A] as a residual quantum yield observed independent of [A]<sup>1</sup>. Homogeneous self-photo-oxidation also occurs and will obviously be the

same as when  $^1O_2^*$  is produced from another sensitizer. This can be written including encounter complexes with the following reactions in place of reactions 16 and 17 in Scheme 1



N.B. In the absence of any differences in orbital symmetry restrictions  $k_q^g$  and  $k_q^h$  in reactions 16a and 17a are the same as in reactions 12a and 13a. Applying the steady-state approximation to ( $S_0..^1O_2^*$ ) which requires  $k_{-d} \gg k_q^g + k_q^h$  gives

$$\frac{d[\text{Products}]_h}{dt} = \frac{-d[A]_h}{dt} = \frac{k_{\text{dif}} k_q^g}{k_{-d}} [^1O_2^*][A] \\ = k_r^A [^1O_2^*][A] \quad (A.14)$$

i.e.

$$k_r^A = \frac{k_{\text{dif}}}{k_{-d}} k_q^g. \quad (A.15)$$

The overall yield of photo-oxidation is the sum of geminate and homogeneous quantum yield i.e.

$$\phi_{\text{ox}} = \phi_{\text{ox}}^g + \phi_{\text{ox}}^h, \quad (A.16)$$

where the superscript h indicates homogeneous reaction. From Eqs. (A.13) and (A.15) it follows that when  $k_{-d} \gg k_q^g + k_q^h$

$$f_r^g = \frac{k_r^A}{k_{\text{dif}}}. \quad (A.17)$$

Substitution of Eqs. (A.13) and (A.17) in Eq. (A.16) gives

$$\phi_{\text{ox}} = \frac{\phi_{\Delta} k_r^A}{k_{\text{dif}}} + (1-f_r^g) \phi_{\Delta} \frac{k_r^A [A]}{(k_d + (k_r^A + k_q^h)[A])} \quad (A.18)$$

or

$$\frac{1}{\phi_{\text{ox}} - \phi_{\text{ox}}^g} = \frac{1}{(1-f_r^g)\phi_{\Delta}} \left[ \left( 1 + \frac{k_q^h}{k_r^A} \right) + \frac{k_d}{k_r^A [A]} \right]. \quad (A.19)$$

This equation is analogous to Eq. (14) since a plot of  $(\phi_{\text{ox}} - \phi_{\text{ox}}^g)^{-1}$  vs.  $[A]^{-1}$  gives slope/intercept =  $\beta_A$ .

## 13. References to Appendix 1

- <sup>1</sup>Merkel, P. B.; Smith, W. F., Jr., *J. Phys. Chem.* **83**: 2834-40 (1979).
- <sup>2</sup>Wilson, T., *J. Am. Chem. Soc.* **88**: 2898-902 (1966).
- <sup>3</sup>Stevens, B.; Marsh, K. L.; Bartrop, J. A., *J. Phys. Chem.* **85**: 3079-82 (1981).
- <sup>4</sup>Drews, W.; Schmidt, R.; Brauer, H.-D., *Chem. Phys. Lett.* **100**: 466-9 (1983).
- <sup>5</sup>Merkel, P. B.; Kearns, D. R., *J. Am. Chem. Soc.* **94**: 7244-53 (1972).

#### 14. Appendix 2: Self-consistent Averages of $\phi_\Delta$ and $f_\Delta^T$

The overall data set contains 1444  $\phi_\Delta$ 's and 357  $f_\Delta^T$ 's, from which 12 values were excluded for such reasons as their being early estimates for which later, more precise, data are available, suspected solvent impurities, etc. Consistency is to be obtained by selecting a reference value for each sensitizer (S) under each set of conditions. Self-consistent averages are indicated by a bar over the quantity symbol; e.g.  $\bar{f}_\Delta^T(S)$  for  $f_\Delta^T$  and  $\bar{\phi}_\Delta(S)$  for  $\phi_\Delta$ . As many values of  $\phi_\Delta(S)$  and  $f_\Delta^T(S)$  as possible are obtained by averaging appropriate values.

The intention of selecting a value by averaging immediately limits the selections to those cases for which there are two or more values to be averaged (50 cases for  $f_\Delta^T$  and 60 for  $\phi_\Delta$ ). Two further restrictions were used in the selection, first that the values agree with each other, second that they should be independent. The requirement for agreement was implemented as a requirement that the standard deviation of the average be no more than 40% of the average. For two values this requires little better than a factor of two agreement. Independence of the values was taken as a requirement that more than one paper contribute to the average.

The conditions for which averages are taken require separate averages for different sensitizers and for different solvents. Further, for  $\phi_\Delta$  values the oxygen concentrations must match, except for sensitizers identified as type T (see Sec. 4). For type T sensitizers,  $\phi_\Delta$  values of a particular sensitizer and solvent are averaged for all oxygen concentrations. For other sensitizers there are separate averages for air-saturated and for oxygen-saturated solutions, with other oxygen concentrations excluded from the averaging.  $f_\Delta^T$  should be independent of oxygen concentration; thus measurements at all oxygen concentrations are included in one average for the same sensitizer and solvent.

In the overall data set 1005 values of  $\phi_\Delta$  and 67 values of  $f_\Delta^T$  are given as ratios,  $R_f(S,S') = \bar{f}_\Delta^T(S)/\bar{f}_\Delta^T(S')$  and  $R_\phi(S,S') = \bar{\phi}_\Delta(S)/\bar{\phi}_\Delta(S')$ . Absolute values can be derived by multiplying by a reference value for S'. When the author states the value of the ratio, or we can calculate the ratio from the given value and the stated reference value used, we use the ratio for our average values. We take each ratio to be as much a measure of S' relative to S as

it is a measure of S relative to S'. This is important for sensitizers that are usually used as references, but for which few data are directly listed in Tables 1-3 (such as phenazine). For those values which are not directly relative, or for which we can not obtain a ratio, the value reported is used in the average.

The basic average of  $n$  measurements, for each set of conditions, comes from summing three types of terms. First the values for S that are not relative, second those that are reported as relative to S' and third those for which S' is reported as relative to S. A separate sum occurs for each distinct pair of sensitizer and solvent when averaging  $f_\Delta^T$ .

$$n\bar{f}_\Delta^T(S) = \sum f_\Delta^T(S) + \sum' R_f(S,S')\bar{f}_\Delta^T(S') + \sum'' [R_f(S'',S)]^{-1}\bar{f}_\Delta^T(S'') \quad (\text{A.2.1})$$

Equation (A.2.1) gives an average ( $\bar{f}_\Delta^T(S)$ ) in terms of similar averages for S' and S''. We started by calculating a set of  $\bar{f}_\Delta^T$  values from the first term and ratios with guessed values used for the  $\bar{f}_\Delta^T$  (0.5 if nothing else was available.) Thereafter each set of  $\bar{f}_\Delta^T$  values was calculated using the previous set in the right hand side of Eq. (A.2.1). After the first iteration measurements for which there was no  $\bar{f}_\Delta^T(S')$  or  $\bar{f}_\Delta^T(S'')$  average were dropped from the second or third sum. The calculations were iterated until no changes resulted with the  $\bar{f}_\Delta^T$  values retained to three decimal places. A similar set of  $\bar{\phi}_\Delta$  values was calculated for the  $\phi_\Delta$  values and their ratios, with separate values for air-saturated and oxygen-saturated (except for type T sensitizers) solvent for each sensitizer.

When the  $\bar{f}_\Delta^T$ 's and the  $\bar{\phi}_\Delta$ 's were derived separately, values for several sensitizers departed from their experimental relationships as expressed in Eq. (42) for type T sensitizers. Further, several  $\bar{f}_\Delta^T$  averaged to values larger than one. Thus the set of averages was calculated in which  $\bar{\phi}_\Delta$  was used in the calculation of  $\bar{f}_\Delta^T$  and vice versa. Specifically in the first term of Eq. (A.2.1) for type T sensitizers  $f_\Delta^T(S)$  terms were replaced by  $\bar{\phi}_\Delta(S)/\bar{\phi}_T$  if  $\bar{\phi}_T$  was also reported. The corresponding substitution for  $\bar{\phi}_\Delta(S)$  was  $\bar{f}_\Delta^T(S)\bar{\phi}_T$  when calculating  $\bar{\phi}_\Delta$ . Also the restriction that all  $\bar{f}_\Delta^T \leq 1.0$  was placed on the averaging procedure.

The resulting  $\bar{f}_\Delta^T$  and  $\bar{\phi}_\Delta$  values, each with the number of measurements and standard deviation of the average, are shown in Table A.2.1.

Table A.2.1. Average values for  $\bar{\phi}_\Delta$  and  $\bar{f}_\Delta^T$ .

| No. <sup>a</sup> | S                                  | Solvent                          | [O <sub>2</sub> ] | Meas. <sup>b</sup> | $\bar{\phi}_\Delta$ | standard deviation | Meas. <sup>c</sup> | $\bar{f}_\Delta^T$ | standard deviation |
|------------------|------------------------------------|----------------------------------|-------------------|--------------------|---------------------|--------------------|--------------------|--------------------|--------------------|
| 1.1              | 2-ACN                              | C <sub>6</sub> H <sub>6</sub>    |                   | 4                  | 0.71                | 0.04               | 4                  | 0.81               | 0.07               |
| 1.2              | AP                                 | C <sub>6</sub> H <sub>6</sub>    |                   | 5                  | 0.36                | 0.007              | 5                  | 0.36               | 0.04               |
| 1.7              | Ac                                 | C <sub>6</sub> H <sub>6</sub>    |                   | 3                  | 0.83                | 0.06               | 5                  | 0.99               | 0.02               |
| 1.13             | An                                 | C <sub>6</sub> H <sub>6</sub>    | air               | 3                  | 0.66                | 0.07               | 2                  | 0.79               | 0.13               |
| 1.13             | An                                 | C <sub>6</sub> H <sub>6</sub>    | O <sub>2</sub>    | 2                  | 0.68                | 0.007              |                    |                    |                    |
| 1.88             | BP                                 | C <sub>6</sub> H <sub>6</sub>    |                   | 9                  | 0.36                | 0.02               | 18                 | 0.35               | 0.03               |
| 1.88             | BP                                 | C <sub>6</sub> D <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.29               | 0.003              |
| 1.115            | Biph                               | C <sub>6</sub> H <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.55               | 0.07               |
| 1.142            | ES                                 | C <sub>6</sub> H <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.96               | 0.05               |
| 1.153            | Fluorenone                         | C <sub>6</sub> H <sub>6</sub>    |                   | 4                  | 0.82                | 0.04               | 3                  | 0.85               | 0.05               |
| 1.161            | Eos                                | H <sub>2</sub> O                 |                   | 3                  | 0.61                | 0.02               |                    |                    |                    |
| 1.161            | Eos                                | EtOH                             |                   |                    |                     |                    | 2                  | 0.78               | 0.20               |
| 1.169            | RB                                 | MeOH                             |                   | 6                  | 0.80                | 0.02               |                    |                    |                    |
| 1.169            | RB                                 | H <sub>2</sub> O                 |                   | 3                  | 0.76                | 0.02               |                    |                    |                    |
| 1.190            | Ery                                | H <sub>2</sub> O                 |                   | 2                  | 0.69                | 0.03               |                    |                    |                    |
| 1.214            | C <sub>17</sub> aldehyde           | MeOH                             |                   | 2                  | 0.41                | 0.00               | 2                  | 1.0                | 0.0                |
| 1.214            | C <sub>17</sub> aldehyde           | c-C <sub>6</sub> H <sub>12</sub> |                   | 2                  | 0.66                | 0.00               | 2                  | 1.0                | 0.0                |
| 1.220            | Np                                 | C <sub>6</sub> H <sub>6</sub>    |                   |                    |                     |                    | 9                  | 0.62               | 0.06               |
| 1.220            | Np                                 | C <sub>6</sub> D <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.49               | 0.005              |
| 1.233            | Per                                | C <sub>6</sub> H <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.93               | 0.09               |
| 1.239            | Pz                                 | C <sub>6</sub> H <sub>6</sub>    |                   | 14                 | 0.88                | 0.07               | 2                  | 1.00               | 0.00               |
| 1.245            | MB <sup>+</sup>                    | MeOH                             |                   | 4                  | 0.51                | 0.01               |                    |                    |                    |
| 1.245            | MB <sup>+</sup>                    | H <sub>2</sub> O                 |                   | 4                  | 0.55                | 0.03               |                    |                    |                    |
| 1.245            | MB <sup>+</sup>                    | EtOH                             |                   |                    |                     |                    | 2                  | 1.00               | 0.0                |
| 1.263            | Py                                 | MeOH                             | O <sub>2</sub>    | 4                  | 0.65                | 0.08               |                    |                    |                    |
| 1.272            | Ret                                | MeOH                             |                   | 2                  | 0.12                | 0.00               | 2                  | 1.00               | 0.0                |
| 1.272            | Ret                                | c-C <sub>6</sub> H <sub>12</sub> |                   |                    |                     |                    | 2                  | 1.00               | 0.0                |
| 1.277            | Rubi                               | C <sub>6</sub> H <sub>6</sub>    | air               | 2                  | 0.27                | 0.05               |                    |                    |                    |
| 1.278            | Rub                                | n-C <sub>6</sub> H <sub>14</sub> | O <sub>2</sub>    | 2                  | 1.17                | 0.05               |                    |                    |                    |
| 1.291            | Tetr                               | C <sub>6</sub> H <sub>6</sub>    | air               | 2                  | 0.69                | 0.01               |                    |                    |                    |
| 1.301            | Thiouridine                        | CH <sub>3</sub> CN               |                   |                    |                     |                    | 4                  | 0.81               | 0.15               |
| 1.306            | Ru(bpy) <sub>3</sub> <sup>2+</sup> | MeOH                             |                   | 4                  | 0.90                | 0.0                | 4                  | 0.95               | 0.0                |
| 1.310            | VD <sub>3</sub>                    | C <sub>6</sub> H <sub>6</sub>    |                   |                    |                     |                    | 2                  | 0.29               | 0.01               |
| 1.316            | Xanthone                           | C <sub>6</sub> H <sub>6</sub>    |                   | 3                  | 0.27                | 0.02               | 3                  | 0.29               | 0.03               |
| 2.12             | Ph a                               | CCl <sub>4</sub>                 | air               | 2                  | 0.74                | 0.04               |                    |                    |                    |
| 2.136            | TPP                                | C <sub>6</sub> H <sub>6</sub>    | air               | 5                  | 0.66                | 0.08               |                    |                    |                    |
| 2.136            | TPP                                | CCl <sub>4</sub>                 | air               | 4                  | 0.62                | 0.07               |                    |                    |                    |
| 2.146            | ZnTPP                              | C <sub>6</sub> H <sub>6</sub>    |                   | 4                  | 0.72                | 0.08               |                    |                    |                    |
| 2.154            | HP                                 | H <sub>2</sub> O                 |                   |                    |                     |                    | 2                  | 0.58               | 0.10               |
| 2.154            | HP                                 | D <sub>2</sub> O (mic)           |                   |                    |                     |                    | 2                  | 0.32               | 0.00               |
| 2.166            | PPDME                              | C <sub>6</sub> D <sub>6</sub>    |                   |                    |                     |                    | 3                  | 0.68               | 0.00               |
| 2.166            | PPDME                              | C <sub>3</sub> H <sub>5</sub> N  | O <sub>2</sub>    | 2                  | 0.90                | 0.28               |                    |                    |                    |

<sup>a</sup>Entry numbers in Tables 1 and 2.<sup>b</sup>Number of measurements of  $\bar{\phi}_\Delta$  in  $\bar{\phi}_\Delta$ .<sup>c</sup>Number of measurements of  $\bar{f}_\Delta^T$  in  $\bar{f}_\Delta^T$ .